p-Terphenyl-d14

Other names: 1,1':4',1''-terphenyl-d14
[2H14]Terphenyl
Inchi: InChI=1S/C18H14/c1-3-7-15(8-4-1)17-11-13-18(14-12-17)16-9-5-2-6-10-16/h1-14H/i1D,2
InchiKey: XJKSTNDFUHDPQJ-WZAAGXFHSA-N
Formula: C18D14
SMILES: c1ccc(-c2ccc(-c3ccccc3)cc2)cc1
Mol. weight [g/mol]: 244.39
CAS: 1718-51-0

Physical Properties

Property code	Value	Unit	Source
gf	428.28	kJ/mol	Joback Method
hf	283.27	kJ/mol	Joback Method
hfus	24.11	kJ/mol	Joback Method
hvap	99.50 ± 4.40	kJ/mol	NIST Webbook
hvap	101.60	kJ/mol	NIST Webbook
log10ws	-6.68		Crippen Method
logp	5.021		Crippen Method
mcvol	193.200	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	358.20		NIST Webbook
ss	315.23	J/mol×K	NIST Webbook
tb	696.26	K	Joback Method
tc	966.50	K	Joback Method
tf	384.40	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.81	J/mol×K	966.50	Joback Method
cpg	570.80	J/mol×K	921.46	Joback Method
cpg	558.66	J/mol×K	876.42	Joback Method
cpg	545.25	J/mol×K	831.38	Joback Method

cpg	530.44	J/mol×K	786.34	Joback Method
cpg	514.08	J/mol×K	741.30	Joback Method
cpg	496.03	J/mol×K	696.26	Joback Method
cps	319.66	J/mol×K	298.15	NIST Webbook
dvisc	0.0001244	Pa×s	696.26	Joback Method
dvisc	0.0013626	Pa×s	384.40	Joback Method
dvisc	0.0007210	Pa×s	436.38	Joback Method
dvisc	0.0004368	Pa×s	488.35	Joback Method
dvisc	0.0002915	Pa×s	540.33	Joback Method
dvisc	0.0002088	Pa×s	592.31	Joback Method
dvisc	0.0001578	Pa×s	644.28	Joback Method
hvapt	101.57	kJ/mol	298.00	Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects
pvap	0.09	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.83e-03	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.90e-03	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	8.07e-04	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	0.02	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.03	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.05	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.36e-04	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.15	kPa	440.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.24	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.37	kPa	460.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	0.57	kPa	470.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.85	kPa	480.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.24	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.76	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.47	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.31e-04	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.73e-05	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	1.57e-05	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.81e-06	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.33e-06	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.04e-06	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	7.93e-03	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons: Liquid Vapor Pressure Isotope Effects:	https://www.doi.org/10.1021/je800091s
Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons:	https://www.doi.org/10.1021/je800300x
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1718510&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume