Benzene, 1,2,4,5-tetrakis(1-methylethyl)-

Other names: 1,2,4,5-Tetraisopropylbenzene
Benzene, 1,2,4,5-tetraisopropyl-
Tetraisopropylbenzene
Inchi: InChI=1S/C18H30/c1-11(2)15-9-17(13(5)6)18(14(7)8)10-16(15)12(3)4/h9-14H,1-8H3
InchiKey: ROXLYQQDLJJEBE-UHFFFAOYSA-N
Formula: C18H30
SMILES: CC(C)c1cc(C(C)C)c(C(C)C)cc1C(C)C
Mol. weight [g/mol]: 246.43
CAS: 635-11-0

Physical Properties

Property code	Value	Unit	Source
gf	174.44	kJ/mol	Joback Method
hf	-233.85	kJ/mol	Joback Method
hfus	21.16	kJ/mol	Joback Method
hvap	58.37	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	6.180		Crippen Method
mcvol	240.720	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	1406.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1569.60		NIST Webbook
tb	651.10	K	Joback Method
tc	852.59	K	Joback Method
tf	412.00 ± 1.50	K	NIST Webbook
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.01	J/mol×K	651.10	Joback Method
cpg	676.73	J/mol×K	684.68	Joback Method

cpg	696.35	J/mol×K	718.26	Joback Method
cpg	714.91	J/mol×K	751.84	Joback Method
cpg	732.44	J/mol×K	785.42	Joback Method
cpg	748.98	J/mol×K	819.01	Joback Method
cpg	764.56	J/mol×K	852.59	Joback Method
dvisc	0.0000889	Pa×s	651.10	Joback Method
dvisc	0.0011945	Pa×s	355.68	Joback Method
dvisc	0.0037365	Pa×s	296.60	Joback Method
dvisc	0.0002865	Pa×s	473.85	Joback Method
dvisc	0.0001779	Pa×s	532.93	Joback Method
dvisc	0.0001215	Pa×s	592.02	Joback Method
dvisc	0.0005285	Pa×s	414.77	Joback Method
hfust	19.60	kJ/mol	393.00	NIST Webbook
hvapt	61.10 ± 0.30	kJ/mol	492.50	NIST Webbook
hvapt	56.80 ± 0.30	kJ/mol	492.50	NIST Webbook
hvapt	52.30 ± 0.50	kJ/mol	492.50	NIST Webbook
hvapt	47.50 ± 0.90	kJ/mol	492.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	488.70	K	9.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.14453e+01
Coeff. B	-3.47153e+03
Coeff. C	-8.90880e+01
Temperature range (K), min.	400.15
Temperature range (K), max.	655.15

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C635110&Units=SI

Legend

cpg:	Ideal gas 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
hfust:	Enthalpy of fusion at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume