1,1-Diphenylpentane

Inchi: InChI=1S/C17H20/c1-2-3-14-17(15-10-6-4-7-11-15)16-12-8-5-9-13-16/h4-13,17H,2-3,14H
InchiKey: GSGNVNZDHCKRGI-UHFFFAOYSA-N
Formula: C17H20
SMILES: CCCCC(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 224.35
CAS: 1726-12-1

Physical Properties

Property code	Value	Unit	Source
af	0.5013		Cheméo Relay (1.0)
chl	-9602.00	kJ/mol	NIST Webbook
gf	314.64	kJ/mol	Joback Method
hf	99.87	kJ/mol	Cheméo Relay (1.0)
hfus	24.34	kJ/mol	Joback Method
hvap	74.92	kJ/mol	Cheméo Relay (1.0)
ie	8.61	eV	Cheméo Relay (1.0)
log10ws	-5.73		Cheméo Relay (1.0)
logp	5.009		Crippen Method
mcvol	202.870	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
tb	581.04 ± 0.30	K	NIST Webbook
tb	581.04 ± 0.30	K	NIST Webbook
tc	808.43	K	Cheméo Relay (1.0)
tf	261.09 ± 0.05	K	NIST Webbook
tf	261.09 ± 0.05	K	NIST Webbook
vc	0.740	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.86	J/mol×K	641.28	Joback Method
cpg	544.30	J/mol×K	679.67	Joback Method
cpg	562.34	J/mol×K	718.05	Joback Method
cpg	579.06	J/mol×K	756.44	Joback Method

cpg	594.56	J/mol×K	794.83	Joback Method
cpg	608.90	J/mol×K	833.21	Joback Method
cpg	622.17	J/mol×K	871.60	Joback Method
dvisc	0.0030325	Pa×s	319.19	Joback Method
dvisc	0.0012216	Pa×s	372.87	Joback Method
dvisc	0.0006186	Pa×s	426.55	Joback Method
dvisc	0.0003648	Pa×s	480.24	Joback Method
dvisc	0.0002392	Pa×s	533.92	Joback Method
dvisc	0.0001694	Pa×s	587.60	Joback Method
dvisc	0.0001271	Pa×s	641.28	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35694e+01
Coeff. B	-4.39699e+03
Coeff. C	-1.02679e+02
Temperature range (K), min.	433.73
Temperature range (K), max.	635.13

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1726121&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor

chl:	Standard liquid enthalpy of combustion
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
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume