1,1-Diphenylhexane

Inchi: InChI=1S/C18H22/c1-2-3-6-15-18(16-11-7-4-8-12-16)17-13-9-5-10-14-17/h4-5,7-14,18H,
InchiKey: BXINIXQKBCSKKR-UHFFFAOYSA-N
Formula: C18H22
SMILES: CCCCCC(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 238.37
CAS: 1530-04-7

Physical Properties

Property code	Value	Unit	Source
af	0.5449		Cheméo Relay (1.0)
chl	-10230.00	kJ/mol	NIST Webbook
gf	323.06	kJ/mol	Joback Method
hf	80.87	kJ/mol	Cheméo Relay (1.0)
hfus	26.94	kJ/mol	Joback Method
hvap	78.84	kJ/mol	Cheméo Relay (1.0)
ie	8.61	eV	Cheméo Relay (1.0)
log10ws	-6.15		Cheméo Relay (1.0)
logp	5.399		Crippen Method
mcvol	216.960	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
tb	594.18 ± 0.30	K	NIST Webbook
tb	594.18 ± 0.30	K	NIST Webbook
tc	819.50	K	Cheméo Relay (1.0)
tf	261.39 ± 0.10	K	NIST Webbook
tf	261.39 ± 0.10	K	NIST Webbook
vc	0.795	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.29	J/mol×K	664.16	Joback Method
cpg	597.96	J/mol×K	701.82	Joback Method
cpg	616.23	J/mol×K	739.48	Joback Method
cpg	633.21	J/mol×K	777.13	Joback Method

cpg	648.97	J/mol×K	814.79	Joback Method
cpg	663.59	J/mol×K	852.45	Joback Method
cpg	677.16	J/mol×K	890.11	Joback Method
dvisc	0.0028308	Pa×s	330.46	Joback Method
dvisc	0.0011284	Pa×s	386.08	Joback Method
dvisc	0.0005670	Pa×s	441.69	Joback Method
dvisc	0.0003323	Pa×s	497.31	Joback Method
dvisc	0.0002169	Pa×s	552.93	Joback Method
dvisc	0.0001530	Pa×s	608.54	Joback Method
dvisc	0.0001145	Pa×s	664.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43785e+01
Coeff. B	-4.76150e+03
Coeff. C	-1.06332e+02
Temperature range (K), min.	444.15
Temperature range (K), max.	631.15

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1530047&Units=SI

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

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

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