1,2-Diphenylbutane

Inchi: InChI=1S/C16H18/c1-2-15(16-11-7-4-8-12-16)13-14-9-5-3-6-10-14/h3-12,15H,2,13H2,1H
InchiKey: XJGHNXQUBBXYCH-UHFFFAOYSA-N
Formula: C16H18
SMILES: CCC(Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 210.31
CAS: 5223-59-6

Physical Properties

Property code	Value	Unit	Source
af	0.4525		Cheméo Relay (1.0)
chl	-8891.00	kJ/mol	NIST Webbook
gf	306.22	kJ/mol	Joback Method
hf	107.42	kJ/mol	Cheméo Relay (1.0)
hfus	21.76	kJ/mol	Joback Method
hvap	77.65	kJ/mol	Cheméo Relay (1.0)
ie	8.38	eV	Cheméo Relay (1.0)
log10ws	-5.11		Cheméo Relay (1.0)
logp	4.423		Crippen Method
mcvol	188.780	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
tb	665.67 ± 0.20	K	NIST Webbook
tb	665.67 ± 0.20	K	NIST Webbook
tc	798.22	K	Cheméo Relay (1.0)
tf	294.25	K	Cheméo Relay (1.0)
vc	0.688	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.73	J/mol×K	618.40	Joback Method
cpg	568.06	J/mol×K	853.40	Joback Method
cpg	555.14	J/mol×K	814.23	Joback Method
cpg	541.15	J/mol×K	775.06	Joback Method
cpg	525.99	J/mol×K	735.90	Joback Method

cpg	509.59	J/mol×K	696.73	Joback Method
cpg	491.86	J/mol×K	657.57	Joback Method
dvisc	0.0003975	Pa×s	463.16	Joback Method
dvisc	0.0001403	Pa×s	618.40	Joback Method
dvisc	0.0001863	Pa×s	566.65	Joback Method
dvisc	0.0002620	Pa×s	514.91	Joback Method
dvisc	0.0032193	Pa×s	307.92	Joback Method
dvisc	0.0006698	Pa×s	411.41	Joback Method
dvisc	0.0013116	Pa×s	359.67	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34629e+01
Coeff. B	-4.24557e+03
Coeff. C	-9.79840e+01
Temperature range (K), min.	420.22
Temperature range (K), max.	618.82

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5223596&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