1,1-Diphenylbutane

Inchi: InChI=1S/C16H18/c1-2-9-16(14-10-5-3-6-11-14)15-12-7-4-8-13-15/h3-8,10-13,16H,2,9H
InchiKey: SZFDQMKAGLCYPA-UHFFFAOYSA-N
Formula: C16H18
SMILES: CCCC(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 210.32
CAS: 719-79-9

Physical Properties

Property code	Value	Unit	Source
af	0.4567		Cheméo Relay (1.0)
chl	-8912.00	kJ/mol	NIST Webbook
chl	-8901.50	kJ/mol	NIST Webbook
gf	306.22	kJ/mol	Joback Method
hf	120.14	kJ/mol	Cheméo Relay (1.0)
hfus	21.76	kJ/mol	Joback Method
hvap	77.20 ± 0.60	kJ/mol	NIST Webbook
ie	8.62	eV	Cheméo Relay (1.0)
log10ws	-5.29		Cheméo Relay (1.0)
logp	4.619		Crippen Method
mcvol	188.780	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
tb	568.44 ± 0.20	K	NIST Webbook
tb	560.00 ± 4.00	K	NIST Webbook
tb	560.00 ± 4.00	K	NIST Webbook
tb	567.44 ± 0.50	K	NIST Webbook
tb	560.20	K	NIST Webbook
tc	796.49	K	Cheméo Relay (1.0)
tf	248.00 ± 0.30	K	NIST Webbook
vc	0.687	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.14	J/mol×K	814.23	Joback Method

cpg	568.06	J/mol×K	853.40	Joback Method
cpg	491.86	J/mol×K	657.57	Joback Method
cpg	509.59	J/mol×K	696.73	Joback Method
cpg	525.99	J/mol×K	735.90	Joback Method
cpg	541.15	J/mol×K	775.06	Joback Method
cpg	472.73	J/mol×K	618.40	Joback Method
dvisc	0.0006698	Pa×s	411.41	Joback Method
dvisc	0.0013116	Pa×s	359.67	Joback Method
dvisc	0.0032193	Pa×s	307.92	Joback Method
dvisc	0.0003975	Pa×s	463.16	Joback Method
dvisc	0.0002620	Pa×s	514.91	Joback Method
dvisc	0.0001863	Pa×s	566.65	Joback Method
dvisc	0.0001403	Pa×s	618.40	Joback Method
hvapt	75.90 ± 0.60	kJ/mol	320.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41152e+01
Coeff. B	-4.40732e+03
Coeff. C	-9.61180e+01
Temperature range (K), min.	414.85
Temperature range (K), max.	596.74

Sources

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=C719799&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):

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
hvapt:	Enthalpy of vaporization at a given temperature
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