

1,1-Dicyclohexylbutane

Other names:	Cyclohexane, 1,1'-butylidenebis-
Inchi:	InChI=1S/C16H30/c1-2-9-16(14-10-5-3-6-11-14)15-12-7-4-8-13-15/h14-16H,2-13H2,1H3
InchiKey:	HYUXMTCTXARFET-UHFFFAOYSA-N
Formula:	C16H30
SMILES:	CCCC(C1CCCCC1)C1CCCCC1
Mol. weight [g/mol]:	222.41
CAS:	54890-00-5

Physical Properties

Property code	Value	Unit	Source
chl	-10220.00	kJ/mol	NIST Webbook
gf	130.30	kJ/mol	Joback Method
hf	-270.21	kJ/mol	Joback Method
hfus	17.34	kJ/mol	Joback Method
hvap	51.68	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	5.563		Crippen Method
mcvol	214.580	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
tb	554.00 ± 6.00	K	NIST Webbook
tb	554.00 ± 6.00	K	NIST Webbook
tb	566.12 ± 1.00	K	NIST Webbook
tc	824.40	K	Joback Method
tf	262.69 ± 0.10	K	NIST Webbook
vc	0.791	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.49	J/mol×K	604.14	Joback Method
cpg	628.82	J/mol×K	640.85	Joback Method
cpg	654.44	J/mol×K	677.56	Joback Method
cpg	678.42	J/mol×K	714.27	Joback Method
cpg	700.82	J/mol×K	750.98	Joback Method

cpg	721.69	J/mol×K	787.69	Joback Method
cpg	741.10	J/mol×K	824.40	Joback Method
dvisc	0.0121478	Paxs	269.84	Joback Method
dvisc	0.0031999	Paxs	325.56	Joback Method
dvisc	0.0012448	Paxs	381.27	Joback Method
dvisc	0.0006161	Paxs	436.99	Joback Method
dvisc	0.0003575	Paxs	492.71	Joback Method
dvisc	0.0002317	Paxs	548.42	Joback Method
dvisc	0.0001627	Paxs	604.14	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.39494e+01
Coeff. B	-4.36309e+03
Coeff. C	-9.85310e+01
Temperature range (K), min.	417.90
Temperature range (K), max.	603.64

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54890005&Units=SI
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/ci9903071
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

Legend

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
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

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