

Cyclohexane, 1,1'-(1-methylpropylidene)bis-

Other names:

Cyclohexane, 1,1'-(1-methylpropylidene)bis-

Inchi:

InChI=1S/C16H30/c1-3-16(2,14-10-6-4-7-11-14)15-12-8-5-9-13-15/h14-15H,3-13H2,1-2H

InchiKey:

AXABZNLJYTXFRF-UHFFFAOYSA-N

Formula:

C16H30

SMILES:

CCC(C)(C1CCCCC1)C1CCCCC1

Mol. weight [g/mol]:

222.42

Physical Properties

Property code	Value	Unit	Source
af	0.3734		Cheméo Relay (1.0)
chl	-10240.00	kJ/mol	NIST Webbook
gf	135.58	kJ/mol	Joback Method
hf	-247.00	kJ/mol	Cheméo Relay (1.0)
hfus	13.45	kJ/mol	Joback Method
hvap	68.29	kJ/mol	Cheméo Relay (1.0)
ie	8.99	eV	Cheméo Relay (1.0)
logp	5.563		Crippen Method
mcvol	214.580	ml/mol	McGowan Method
pc	1849.92	kPa	Joback Method
tb	575.30 ± 0.60	K	NIST Webbook
tb	575.30 ± 0.60	K	NIST Webbook
tc	783.54	K	Cheméo Relay (1.0)
tf	288.53 ± 0.10	K	NIST Webbook
tf	288.53 ± 0.10	K	NIST Webbook
vc	0.743	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.44	J/mol×K	601.35	Joback Method
cpg	631.74	J/mol×K	639.52	Joback Method
cpg	658.11	J/mol×K	677.69	Joback Method
cpg	682.64	J/mol×K	715.85	Joback Method
cpg	705.42	J/mol×K	754.02	Joback Method

cpg	726.54	J/mol×K	792.19	Joback Method
cpg	746.10	J/mol×K	830.36	Joback Method
dvisc	0.0102795	Pa×s	287.26	Joback Method
dvisc	0.0029824	Pa×s	339.61	Joback Method
dvisc	0.0012042	Pa×s	391.96	Joback Method
dvisc	0.0006021	Pa×s	444.31	Joback Method
dvisc	0.0003484	Pa×s	496.65	Joback Method
dvisc	0.0002238	Pa×s	549.00	Joback Method
dvisc	0.0001552	Pa×s	601.35	Joback Method

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54890027&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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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