

Cyclohexane, 1,1'-(1,4-butanediyl)bis-

Other names:	1,4-Dicyclohexylbutane Butane, 1,4-dicyclohexyl-
Inchi:	InChI=1S/C16H30/c1-3-9-15(10-4-1)13-7-8-14-16-11-5-2-6-12-16/h15-16H,1-14H2
InchiKey:	UWSSRUCETFDRLMI-UHFFFAOYSA-N
Formula:	C16H30
SMILES:	C1CCC(CCCCC2CCCCC2)CC1
Mol. weight [g/mol]:	222.41
CAS:	6165-44-2

Physical Properties

Property code	Value	Unit	Source
gf	132.74	kJ/mol	Joback Method
hf	-264.93	kJ/mol	Joback Method
hfus	20.87	kJ/mol	Joback Method
hvap	52.07	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.707		Crippen Method
mcvol	214.580	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	1699.00		NIST Webbook
tb	604.58	K	Joback Method
tc	820.33	K	Joback Method
tf	284.84	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.21	J/mol×K	604.58	Joback Method
cpg	627.93	J/mol×K	640.54	Joback Method
cpg	653.02	J/mol×K	676.50	Joback Method
cpg	676.54	J/mol×K	712.45	Joback Method
cpg	698.56	J/mol×K	748.41	Joback Method
cpg	719.11	J/mol×K	784.37	Joback Method

cpg	738.27	J/mol×K	820.33	Joback Method
dvisc	0.0080678	Pa×s	284.84	Joback Method
dvisc	0.0025729	Pa×s	338.13	Joback Method
dvisc	0.0011200	Pa×s	391.42	Joback Method
dvisc	0.0005951	Pa×s	444.71	Joback Method
dvisc	0.0003620	Pa×s	498.00	Joback Method
dvisc	0.0002425	Pa×s	551.29	Joback Method
dvisc	0.0001743	Pa×s	604.58	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.39902e+01
Coeff. B	-4.46217e+03
Coeff. C	-1.01876e+02
Temperature range (K), min.	427.52
Temperature range (K), max.	616.03

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6165442&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/ci990307l
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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