

Cyclohexane, 1,1'-methylenebis-

Other names:	Dicyclohexylmethane Methane, dicyclohexyl-
Inchi:	InChI=1S/C13H24/c1-3-7-12(8-4-1)11-13-9-5-2-6-10-13/h12-13H,1-11H2
InchiKey:	XXKOQQBKBHUATC-UHFFFAOYSA-N
Formula:	C13H24
SMILES:	C1CCC(CC2CCCCC2)CC1
Mol. weight [g/mol]:	180.33
CAS:	3178-23-2

Physical Properties

Property code	Value	Unit	Source
chl	-8170.45	kJ/mol	NIST Webbook
chl	-8250.80	kJ/mol	NIST Webbook
chl	-7719.00	kJ/mol	NIST Webbook
gf	107.48	kJ/mol	Joback Method
hf	-203.01	kJ/mol	Joback Method
hfus	13.10	kJ/mol	Joback Method
hvap	45.39	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.537		Crippen Method
mcvol	172.310	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinpol	1427.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1385.00		NIST Webbook
tb	526.00 ± 0.60	K	NIST Webbook
tb	525.92 ± 1.00	K	NIST Webbook
tb	525.00 ± 3.00	K	NIST Webbook
tb	523.00 ± 2.00	K	NIST Webbook
tb	524.00 ± 3.00	K	NIST Webbook
tc	763.72	K	Joback Method
tf	254.46 ± 0.30	K	NIST Webbook
tf	254.45 ± 0.30	K	NIST Webbook
tf	254.45 ± 0.20	K	NIST Webbook
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.88	J/mol×K	535.94	Joback Method
cpg	463.27	J/mol×K	573.90	Joback Method
cpg	488.03	J/mol×K	611.87	Joback Method
cpg	511.21	J/mol×K	649.83	Joback Method
cpg	532.87	J/mol×K	687.79	Joback Method
cpg	553.06	J/mol×K	725.76	Joback Method
cpg	571.84	J/mol×K	763.72	Joback Method
cpl	320.10	J/mol×K	313.00	NIST Webbook
cpl	355.20	J/mol×K	311.00	NIST Webbook
dvisc	0.0102425	Pa×s	251.03	Joback Method
dvisc	0.0033091	Pa×s	298.51	Joback Method
dvisc	0.0014578	Pa×s	346.00	Joback Method
dvisc	0.0007827	Pa×s	393.49	Joback Method
dvisc	0.0004805	Pa×s	440.97	Joback Method
dvisc	0.0003243	Pa×s	488.46	Joback Method
dvisc	0.0002347	Pa×s	535.94	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38331e+01
Coeff. B	-4.04191e+03
Coeff. C	-8.73640e+01
Temperature range (K), min.	385.76
Temperature range (K), max.	561.68

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3178232&Units=SI>

The Yaws Handbook of Vapor

Pressure:
Crippen Method:

Crippen Method:

Joback Method:

McGowan Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

https://www.chemeo.com/doc/models/crippen_log10ws

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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