

Cyclohexane, 1,1'-propylidenebis-

Other names:	1,1-Dicyclohexylpropane
Inchi:	InChI=1S/C15H28/c1-2-15(13-9-5-3-6-10-13)14-11-7-4-8-12-14/h13-15H,2-12H2,1H3
InchiKey:	ROFWOEQFASWFTK-UHFFFAOYSA-N
Formula:	C15H28
SMILES:	CCC(C1CCCCC1)C1CCCCC1
Mol. weight [g/mol]:	208.38
CAS:	54934-91-7

Physical Properties

Property code	Value	Unit	Source
chs	-8954.00	kJ/mol	NIST Webbook
gf	121.88	kJ/mol	Joback Method
hf	-249.57	kJ/mol	Joback Method
hfus	14.75	kJ/mol	Joback Method
hvap	49.45	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	5.173		Crippen Method
mcvol	200.490	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
tb	556.71 ± 0.30	K	NIST Webbook
tb	544.00 ± 6.00	K	NIST Webbook
tb	544.00 ± 6.00	K	NIST Webbook
tb	555.46 ± 1.00	K	NIST Webbook
tc	805.62	K	Joback Method
tf	249.69 ± 0.30	K	NIST Webbook
tf	249.69 ± 1.00	K	NIST Webbook
tf	244.84 ± 0.40	K	NIST Webbook
tf	249.69 ± 0.50	K	NIST Webbook
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.31	J/mol×K	581.26	Joback Method

cpg	665.45	J/molxK	768.22	Joback Method
cpg	644.61	J/molxK	730.83	Joback Method
cpg	622.24	J/molxK	693.44	Joback Method
cpg	598.27	J/molxK	656.05	Joback Method
cpg	572.64	J/molxK	618.65	Joback Method
cpg	684.81	J/molxK	805.62	Joback Method
dvisc	0.0001814	Paxs	581.26	Joback Method
dvisc	0.0002580	Paxs	527.48	Joback Method
dvisc	0.0003976	Paxs	473.70	Joback Method
dvisc	0.0006845	Paxs	419.91	Joback Method
dvisc	0.0013823	Paxs	366.13	Joback Method
dvisc	0.0035561	Paxs	312.35	Joback Method
dvisc	0.0135528	Paxs	258.57	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.39240e+01
Coeff. B	-4.28800e+03
Coeff. C	-9.59150e+01
Temperature range (K), min.	410.37
Temperature range (K), max.	593.80

Sources

The Yaws Handbook of Vapor

Pressure:
Crippen Method:

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

<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>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C54934917&Units=SI>

Legend

chs:	Standard solid 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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