

4-Isopropyldicyclohexylmethane

Other names:	Cyclohexane, 1-(cyclohexylmethyl)-4-(1-methylethyl)- Methane, cyclohexyl(4-isopropylcyclohexyl)-
Inchi:	InChI=1S/C16H30/c1-13(2)16-10-8-15(9-11-16)12-14-6-4-3-5-7-14/h13-16H,3-12H2,1-2H3
InchiKey:	LHWJKUKEUOFSME-UHFFFAOYSA-N
Formula:	C16H30
SMILES:	CC(C)C1CCC(CC2CCCCC2)CC1
Mol. weight [g/mol]:	222.41
CAS:	54965-61-6

Physical Properties

Property code	Value	Unit	Source
chs	-10180.00	kJ/mol	NIST Webbook
chs	-10200.00	kJ/mol	NIST Webbook
gf	122.59	kJ/mol	Joback Method
hf	-290.55	kJ/mol	Joback Method
hfus	18.41	kJ/mol	Joback Method
hvap	51.37	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	5.419		Crippen Method
mvol	214.580	ml/mol	McGowan Method
pc	1781.84	kPa	Joback Method
tb	599.47	K	Joback Method
tc	819.72	K	Joback Method
tf	265.60	K	Joback Method
vc	0.790	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.79	J/mol×K	599.47	Joback Method
cpg	629.69	J/mol×K	636.18	Joback Method
cpg	655.89	J/mol×K	672.89	Joback Method
cpg	680.43	J/mol×K	709.60	Joback Method
cpg	703.37	J/mol×K	746.30	Joback Method

cpg	724.75	J/molxK	783.01	Joback Method
cpg	744.63	J/molxK	819.72	Joback Method
dvisc	0.0091891	Paxs	265.60	Joback Method
dvisc	0.0027396	Paxs	321.25	Joback Method
dvisc	0.0011676	Paxs	376.89	Joback Method
dvisc	0.0006197	Paxs	432.53	Joback Method
dvisc	0.0003800	Paxs	488.18	Joback Method
dvisc	0.0002576	Paxs	543.83	Joback Method
dvisc	0.0001876	Paxs	599.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54965616&Units=SI
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

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
mccvol:	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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