Cyclohexane, 1,4-dimethyl-2-(2-methylpropyl)-, (1«alpha»,2«beta»,4«alpha»)-

Other names:	cis,trans,cis-1-Isobutyl-2,5-dimethylcyclohexane Cyclohexane, 1,4-dimethyl-2-(2-methylpropyl)-, (1R,2R,4R)-rel- 2-Isobutyl-1,4-dimethylcyclohexane, (1«alpha»,2«beta»,4«alpha»)- cyclohexane, 1,4-dimethyl-2-(2-methylpropyl)-, (1«beta»,2«alpha»,5«beta»)-
Inchi:	InChI=1S/C12H24/c1-9(2)7-12-8-10(3)5-6-11(12)4/h9-12H,5-8H2,1-4H3
InchiKey:	ZYJPKZNMMTYTPA-UHFFFAOYSA-N
Formula:	C12H24
SMILES:	CC(C)CC1CC(C)CCC1C
Mol. weight [g/mol]:	168.32
CAS:	54411-17-5

Physical Properties

Property code	Value	Unit	Source
gf	56.75	kJ/mol	Joback Method
hf	-282.65	kJ/mol	Joback Method
hfus	17.29	kJ/mol	Joback Method
hvap	41.73	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	4.105		Crippen Method
mcvol	169.080	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
tb	483.73	K	Joback Method
tc	679.68	K	Joback Method
tf	208.90	K	Joback Method
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.76	J/mol×K	483.73	Joback Method
cpg	495.86	J/mol×K	647.02	Joback Method
cpg	477.58	J/mol×K	614.36	Joback Method
cpg	458.35	J/mol×K	581.71	Joback Method
cpg	438.15	J/mol×K	549.05	Joback Method

cpg	416.96	J/mol×K	516.39	Joback Method
cpg	513.20	J/mol×K	679.68	Joback Method
dvisc	0.0002445	Pa×s	483.73	Joback Method
dvisc	0.0003106	Pa×s	437.93	Joback Method
dvisc	0.0004173	Pa×s	392.12	Joback Method
dvisc	0.0006061	Pa×s	346.32	Joback Method
dvisc	0.0009867	Pa×s	300.51	Joback Method
dvisc	0.0019139	Pa×s	254.71	Joback Method
dvisc	0.0049638	Pa×s	208.90	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54411175&Units=SI

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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