Cyclohexane, 1-(1,5-dimethylhexyl)-4-methyl-

Other names:	Heptane, 2-methyl-6-(4-methylcyclohexyl)-
	Bisabolane
	Bisabolene, trans-
Inchi:	InChI=1S/C15H30/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h12-15H,5-11H2,1-4H3
InchiKey:	NOWQRWPUNHMSAF-UHFFFAOYSA-N
Formula:	C15H30
SMILES:	CC(C)CCCC(C)C1CCC(C)CC1
Mol. weight [g/mol]:	210.40
CAS:	29799-19-7

Physical Properties

Property code	Value	Unit	Source
gf	87.28	kJ/mol	Joback Method
hf	-329.51	kJ/mol	Joback Method
hfus	20.47	kJ/mol	Joback Method
hvap	48.33	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	5.275		Crippen Method
mcvol	211.350	ml/mol	McGowan Method
pc	1639.10	kPa	Joback Method
rinpol	1458.00		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1458.00		NIST Webbook
ripol	1521.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1501.00		NIST Webbook
ripol	1510.00		NIST Webbook
tb	556.60	K	Joback Method
tc	749.41	K	Joback Method
tf	231.95	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.45	J/mol×K	556.60	Joback Method
cpg	658.63	J/mol×K	717.28	Joback Method
cpg	639.40	J/mol×K	685.14	Joback Method
cpg	619.10	J/mol×K	653.01	Joback Method
cpg	597.69	J/mol×K	620.87	Joback Method
cpg	575.15	J/mol×K	588.74	Joback Method
cpg	676.81	J/mol×K	749.41	Joback Method
dvisc	0.0001782	Pa×s	556.60	Joback Method
dvisc	0.0002464	Pa×s	502.49	Joback Method
dvisc	0.0003685	Pa×s	448.38	Joback Method
dvisc	0.0006152	Pa×s	394.27	Joback Method
dvisc	0.0012093	Pa×s	340.17	Joback Method
dvisc	0.0030693	Pa×s	286.06	Joback Method
dvisc	0.0120303	Pa×s	231.95	Joback Method

Sources

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=C29799197&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol: Non-polar retention indices
ripol: Polar retention indices

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

Latest version available from:
https://www.chemeo.com/cid/75-176-4/Cyclohexane-1-1-5-dimethylhexyl-4-methyl.pdf
Generated by Cheméo on 2024-04-24 19:27:59.88263879 +0000 UTC m=+16276128.803216112.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.