Cyclohexanol, 2-methyl-5-(1-methylethyl)-, (1«alpha»,2«alpha»,5«alpha»)-

Other names: Neoisocarvomenthol

5-Isopropyl-2-methylcyclohexanol, (1«alpha»,2«alpha»,5«alpha»)-

Inchi: InChI=1S/C10H20O/c1-7(2)9-5-4-8(3)10(11)6-9/h7-11H,4-6H2,1-3H3/t8-,9+,10+/m0/s1

InchiKey: ULJXKUJMXIVDOY-IVZWLZJFSA-N

Formula: C10H20O

SMILES: CC(C)C1CCC(C)C(O)C1

Mol. weight [g/mol]: 156.27

CAS: 42846-32-2

Physical Properties

Property code	Value	Unit	Source
gf	-96.91	kJ/mol	Joback Method
hf	-393.60	kJ/mol	Joback Method
hfus	16.20	kJ/mol	Joback Method
hvap	53.96	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.440		Crippen Method
mcvol	146.770	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
rinpol	1186.00		NIST Webbook
tb	530.15	K	Joback Method
tc	719.67	K	Joback Method
tf	247.18	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.36	J/mol×K	530.15	Joback Method
cpg	449.82	J/mol×K	688.08	Joback Method
cpg	435.50	J/mol×K	656.49	Joback Method
cpg	420.40	J/mol×K	624.91	Joback Method
cpg	404.52	J/mol×K	593.32	Joback Method
cpg	387.84	J/mol×K	561.74	Joback Method

cpg	463.40	J/mol×K	719.67	Joback Method
dvisc	0.0001446	Pa×s	530.15	Joback Method
dvisc	0.0002350	Pa×s	482.99	Joback Method
dvisc	0.0004244	Pa×s	435.83	Joback Method
dvisc	0.0008847	Pa×s	388.66	Joback Method
dvisc	0.0022592	Pa×s	341.50	Joback Method
dvisc	0.0077902	Pa×s	294.34	Joback Method
dvisc	0.0430815	Pa×s	247.18	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C42846322&Units=SI
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

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

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