NEODIHYDROCARVEOL

Other names: neo-iso-Dihydrocarveol
Inchi: InChI=1S/C10H18O/c1-7(2)9-5-4-8(3)10(11)6-9/h8-11H,1,4-6H2,2-3H3
InchiKey: KRCZYMFUWVJCLI-UHFFFAOYSA-N
Formula: C10H18O
SMILES: C=C(C)C1CCC(C)C(O)C1
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
hf	-257.77	kJ/mol	Cheméo Relay (1.0)
hfus	17.13	kJ/mol	Joback Method
hvap	72.13	kJ/mol	Cheméo Relay (1.0)
ie	8.89	eV	Cheméo Relay (1.0)
logp	2.360		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
tb	497.02	K	Cheméo Relay (1.0)
tf	304.28	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.71	J/mol×K	527.15	Joback Method
cpg	367.51	J/mol×K	559.26	Joback Method
cpg	383.50	J/mol×K	591.37	Joback Method
cpg	398.69	J/mol×K	623.47	Joback Method
cpg	413.11	J/mol×K	655.58	Joback Method
cpg	426.76	J/mol×K	687.69	Joback Method
cpg	439.67	J/mol×K	719.80	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18675348&Units=SI
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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