Dehydroxylinalooloxide A

Inchi: InChI=1S/C10H18O/c1-5-10(4)8-6-7-9(2,3)11-10/h5H,1,6-8H2,2-4H3/t10-/m1/s1
InchiKey: NETOHYFTCONTDT-SNVBAGLBSA-N
Formula: C10H18O
SMILES: C=CC1(C)CCCC(C)(C)O1
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	40.80	kJ/mol	Joback Method
hf	-191.84	kJ/mol	Joback Method
hfus	8.66	kJ/mol	Joback Method
hvap	39.51	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.910		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2820.33	kPa	Joback Method
rinpol	977.00		NIST Webbook
rinpol	977.00		NIST Webbook
tb	467.19	K	Joback Method
tc	685.50	K	Joback Method
tf	278.21	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.94	J/mol×K	467.19	Joback Method
cpg	337.17	J/mol×K	503.58	Joback Method
cpg	354.87	J/mol×K	539.96	Joback Method
cpg	371.27	J/mol×K	576.35	Joback Method
cpg	386.55	J/mol×K	612.73	Joback Method
cpg	400.92	J/mol×K	649.12	Joback Method
cpg	414.58	J/mol×K	685.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R288370&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
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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