Dihydroedulan

Inchi: InChI=1S/C13H22O/c1-10-6-7-11-12(2,3)8-5-9-13(11,4)14-10/h5,9-11H,6-8H2,1-4H3
InchiKey: IVTQSEFLDHBCDZ-UHFFFAOYSA-N
Formula: C13H22O
SMILES: CC1CCC2C(C)(C)CC=CC2(C)O1
Mol. weight [g/mol]: 194.31

Physical Properties

Property code	Value	Unit	Source
gf	49.12	kJ/mol	Joback Method
hf	-275.11	kJ/mol	Joback Method
hfus	16.04	kJ/mol	Joback Method
hvap	46.93	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.546		Crippen Method
mcvol	173.880	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
rinpol	1306.00		NIST Webbook
rinpol	1306.00		NIST Webbook
ripol	1492.00		NIST Webbook
ripol	1492.00		NIST Webbook
tb	544.65	K	Joback Method
tc	774.56	K	Joback Method
tf	324.72	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.15	J/mol×K	544.65	Joback Method
cpg	473.87	J/mol×K	582.97	Joback Method
cpg	494.99	J/mol×K	621.29	Joback Method
cpg	514.78	J/mol×K	659.61	Joback Method
cpg	533.50	J/mol×K	697.93	Joback Method
cpg	551.39	J/mol×K	736.24	Joback Method

cpg	568.71	J/mol×K	774.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R330233&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume