9-oxo-Dihydroedulan II

Inchi: InChI=1S/C13H20O2/c1-9-8-10(14)11-12(2,3)6-5-7-13(11,4)15-9/h5,7,9,11H,6,8H2,1-4H
InchiKey: MWMVBTVTTIYZCK-NTPLCPOISA-N
Formula: C13H20O2
SMILES: CC1CC(=O)C2C(C)(C)CC=CC2(C)O1
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	-73.47	kJ/mol	Joback Method
hf	-412.81	kJ/mol	Joback Method
hfus	15.55	kJ/mol	Joback Method
hvap	51.17	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.725		Crippen Method
mcvol	175.450	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	1488.10		NIST Webbook
tb	612.47	K	Joback Method
tc	856.32	K	Joback Method
tf	392.94	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.18	J/mol×K	612.47	Joback Method
cpg	510.62	J/mol×K	653.11	Joback Method
cpg	530.88	J/mol×K	693.75	Joback Method
cpg	550.21	J/mol×K	734.39	Joback Method
cpg	568.88	J/mol×K	775.04	Joback Method
cpg	587.13	J/mol×K	815.68	Joback Method
cpg	605.24	J/mol×K	856.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R416332&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