9-oxo-Tetrahydroedulan I

Inchi: InChI=1S/C13H22O2/c1-9-8-10(14)11-12(2,3)6-5-7-13(11,4)15-9/h9,11H,5-8H2,1-4H3/t9
InchiKey: QFHNUZLPOUYWJG-XTLKWQJWSA-N
Formula: C13H22O2
SMILES: CC1CC(=O)C2C(C)(C)CCCC2(C)O1
Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
gf	-103.43	kJ/mol	Joback Method
hf	-470.59	kJ/mol	Joback Method
hfus	14.33	kJ/mol	Joback Method
hvap	50.88	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.949		Crippen Method
mcvol	179.750	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinpol	1516.20		NIST Webbook
tb	613.31	K	Joback Method
tc	854.77	K	Joback Method
tf	392.18	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.45	J/mol×K	613.31	Joback Method
cpg	533.06	J/mol×K	653.55	Joback Method
cpg	554.45	J/mol×K	693.80	Joback Method
cpg	574.86	J/mol×K	734.04	Joback Method
cpg	594.54	J/mol×K	774.28	Joback Method
cpg	613.74	J/mol×K	814.52	Joback Method
cpg	632.72	J/mol×K	854.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R416347&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

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