4-Oxo-«beta»-isodamascol

Inchi: InChI=1S/C13H20O2/c1-8(2)12(15)11-9(3)10(14)6-7-13(11,4)5/h12,15H,1,6-7H2,2-5H3
InchiKey: SLCFYYKEJSZUCI-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: C=C(C)C(O)C1=C(C)C(=O)CCC1(C)C
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	-94.32	kJ/mol	Joback Method
hf	-386.82	kJ/mol	Joback Method
hfus	12.89	kJ/mol	Joback Method
hvap	65.37	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.629		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1753.00		NIST Webbook
rinpol	1753.00		NIST Webbook
tb	681.87	K	Joback Method
tc	893.36	K	Joback Method
tf	391.67	K	Joback Method
vc	0.682	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.77	J/mol×K	681.87	Joback Method
cpg	524.65	J/mol×K	717.12	Joback Method
cpg	539.86	J/mol×K	752.37	Joback Method
cpg	554.46	J/mol×K	787.62	Joback Method
cpg	568.55	J/mol×K	822.87	Joback Method
cpg	582.22	J/mol×K	858.12	Joback Method
cpg	595.54	J/mol×K	893.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U108911&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