Cyclohexanemalonic acid, 4,4-dimethyl-alpha-hydroxy-2-(1-hydroxyethyl)-,ga

Inchi: InChI=1S/C13H18O4/c1-6-8-5-13(2,3)9-4-7(8)10(11(14)16-6)12(15)17-9/h6-10H,4-5H2,1

InchiKey: FSZHUBKZXLBHGH-UHFFFAOYSA-N

Formula: C13H18O4

SMILES: CC1OC(=O)C2C(=O)OC3CC2C1CC3(C)C

Mol. weight [g/mol]: 238.28

Physical Properties

Property code	Value	Unit	Source
gf	-241.51	kJ/mol	Joback Method
hf	-696.91	kJ/mol	Joback Method
hfus	29.42	kJ/mol	Joback Method
hvap	60.22	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	1.526		Crippen Method
mcvol	176.330	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
tb	705.64	K	Joback Method
tc	954.61	K	Joback Method
tf	480.29	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.26	J/mol×K	705.64	Joback Method
cpg	590.37	J/mol×K	747.14	Joback Method
cpg	610.33	J/mol×K	788.63	Joback Method
cpg	629.27	J/mol×K	830.13	Joback Method
cpg	647.34	J/mol×K	871.62	Joback Method
cpg	664.67	J/mol×K	913.12	Joback Method
cpg	681.40	J/mol×K	954.61	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6005267&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume