Cyclohexanemalonic acid, 5-hydroxy-2-(1-hydroxyethyl)-4,4-dimethyl-alpha-[

Inchi: InChI=1S/C18H29NO4/c1-11(10-19(5)6)18-13-9-17(4,23-15(18)21)8-7-12(13)16(2,3)22-1

InchiKey: SSOFRYHMIDPVCV-UHFFFAOYSA-N

Formula: C18H29NO4

SMILES: CC(CN(C)C)C12C(=O)OC3(C)CCC(C1C3)C(C)(C)OC2=O

Mol. weight [g/mol]: 323.43

Physical Properties

Property code	Value	Unit	Source
gf	-94.34	kJ/mol	Joback Method
hf	-687.04	kJ/mol	Joback Method
hfus	28.20	kJ/mol	Joback Method
hvap	71.02	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.238		Crippen Method
mcvol	256.760	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
tb	837.19	K	Joback Method
tc	1079.02	K	Joback Method
tf	606.15	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.50	J/mol×K	837.19	Joback Method
cpg	918.71	J/mol×K	877.49	Joback Method
cpg	945.51	J/mol×K	917.80	Joback Method
cpg	973.31	J/mol×K	958.10	Joback Method
cpg	1002.50	J/mol×K	998.41	Joback Method
cpg	1033.52	J/mol×K	1038.71	Joback Method
cpg	1066.75	J/mol×K	1079.02	Joback Method

Sources

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=B6005279&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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