Ethosuximide, M(HO-ethyl-), AC

Inchi: InChI=1S/C9H13NO4/c1-5(14-6(2)11)9(3)4-7(12)10-8(9)13/h5H,4H2,1-3H3,(H,10,12,13)
InchiKey: HPPSBFDEKMLBAO-UHFFFAOYSA-N
Formula: C9H13NO4
SMILES: CC(=O)OC(C)C1(C)CC(=O)NC1=O
Mol. weight [g/mol]: 199.20

Physical Properties

Property code	Value	Unit	Source
gf	-337.87	kJ/mol	Joback Method
hf	-641.04	kJ/mol	Joback Method
hfus	14.58	kJ/mol	Joback Method
hvap	58.75	kJ/mol	Joback Method
log10ws	-0.96		Crippen Method
logp	-0.009		Crippen Method
mcvol	147.370	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
rinpol	1390.00		NIST Webbook
tb	680.88	K	Joback Method
tc	925.64	K	Joback Method
tf	524.62	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.83	J/mol×K	680.88	Joback Method
cpg	423.24	J/mol×K	721.67	Joback Method
cpg	437.93	J/mol×K	762.47	Joback Method
cpg	451.97	J/mol×K	803.26	Joback Method
cpg	465.39	J/mol×K	844.05	Joback Method
cpg	478.24	J/mol×K	884.84	Joback Method
cpg	490.56	J/mol×K	925.64	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=R255617&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume