Ethosuximide, M(3-HO-), AC

Inchi: InChI=1S/C9H13NO4/c1-4-9(3)6(14-5(2)11)7(12)10-8(9)13/h6H,4H2,1-3H3,(H,10,12,13)
InchiKey: GEENBIYQOOCZCA-UHFFFAOYSA-N
Formula: C9H13NO4
SMILES: CCC1(C)C(=O)NC(=O)C1OC(C)=O
Mol. weight [g/mol]: 199.20

Physical Properties

Property code	Value	Unit	Source
gf	-343.14	kJ/mol	Joback Method
hf	-656.10	kJ/mol	Joback Method
hfus	19.17	kJ/mol	Joback Method
hvap	58.83	kJ/mol	Joback Method
log10ws	-0.96		Crippen Method
logp	-0.009		Crippen Method
mcvol	147.370	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
rinpol	1350.00		NIST Webbook
rinpol	1350.00		NIST Webbook
tb	676.65	K	Joback Method
tc	916.57	K	Joback Method
tf	535.38	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.14	J/mol×K	676.65	Joback Method
cpg	425.68	J/mol×K	716.64	Joback Method
cpg	440.53	J/mol×K	756.62	Joback Method
cpg	454.72	J/mol×K	796.61	Joback Method
cpg	468.29	J/mol×K	836.60	Joback Method
cpg	481.27	J/mol×K	876.59	Joback Method
cpg	493.69	J/mol×K	916.57	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=R255602&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume