Mesuximide, M (nor-HO-) isomer 1, AC

Inchi: InChI=1S/C13H13NO4/c1-8(15)18-10-5-3-9(4-6-10)13(2)7-11(16)14-12(13)17/h3-6H,7H2
InchiKey: DGEYRUVEGABFCW-UHFFFAOYSA-N
Formula: C13H13NO4
SMILES: CC(=O)Oc1ccc(C2(C)CC(=O)NC2=O)cc1
Mol. weight [g/mol]: 247.25

Physical Properties

Property code	Value	Unit	Source
gf	-198.97	kJ/mol	Joback Method
hf	-493.26	kJ/mol	Joback Method
hfus	22.11	kJ/mol	Joback Method
hvap	70.98	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	0.916		Crippen Method
mcvol	179.970	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
rinpol	2120.00		NIST Webbook
rinpol	2120.00		NIST Webbook
tb	804.50	K	Joback Method
tc	1069.47	K	Joback Method
tf	623.64	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.22	J/mol×K	804.50	Joback Method
cpg	546.48	J/mol×K	848.66	Joback Method
cpg	561.87	J/mol×K	892.82	Joback Method
cpg	576.46	J/mol×K	936.99	Joback Method
cpg	590.34	J/mol×K	981.15	Joback Method
cpg	603.59	J/mol×K	1025.31	Joback Method
cpg	616.29	J/mol×K	1069.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R255682&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

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