Glutethimide M (OH-phenyl)

Inchi: InChI=1S/C13H15NO3/c1-2-13(8-7-11(16)14-12(13)17)9-3-5-10(15)6-4-9/h3-6,15H,2,7-8
InchiKey: LJYPZSQFNJDVIO-UHFFFAOYSA-N
Formula: C13H15NO3
SMILES: CCC1(c2ccc(O)cc2)CCC(=O)NC1=O
Mol. weight [g/mol]: 233.26

Physical Properties

Property code	Value	Unit	Source
gf	-122.14	kJ/mol	Joback Method
hf	-420.46	kJ/mol	Joback Method
hfus	23.40	kJ/mol	Joback Method
hvap	74.35	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	1.477		Crippen Method
mcvol	178.400	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
rinpol	2250.00		NIST Webbook
tb	808.12	K	Joback Method
tc	1086.40	K	Joback Method
tf	647.16	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.03	J/mol×K	808.12	Joback Method
cpg	562.82	J/mol×K	854.50	Joback Method
cpg	580.03	J/mol×K	900.88	Joback Method
cpg	596.85	J/mol×K	947.26	Joback Method
cpg	613.51	J/mol×K	993.64	Joback Method
cpg	630.21	J/mol×K	1040.02	Joback Method
cpg	647.16	J/mol×K	1086.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R57452&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