Secobarbital M (OH, -H2O)

Inchi: InChI=1S/C11H14N2O3/c1-4-6-11(7(3)5-2)8(14)12-10(16)13-9(11)15/h4-5H,1,6H2,2-3H3
InchiKey: WPIQHWSPEILYJT-FNORWQNLSA-N
Formula: C11H14N2O3
SMILES: C=CCC1(C(C)=CC)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 222.24

Physical Properties

Property code	Value	Unit	Source
gf	27.86	kJ/mol	Joback Method
hf	-305.43	kJ/mol	Joback Method
hfus	25.11	kJ/mol	Joback Method
hvap	64.98	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	0.881		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook
tb	772.15	K	Joback Method
tc	1038.87	K	Joback Method
tf	638.93	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.76	J/mol×K	772.15	Joback Method
cpg	516.29	J/mol×K	816.60	Joback Method
cpg	532.93	J/mol×K	861.06	Joback Method
cpg	548.72	J/mol×K	905.51	Joback Method
cpg	563.72	J/mol×K	949.97	Joback Method
cpg	577.96	J/mol×K	994.42	Joback Method
cpg	591.50	J/mol×K	1038.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R57644&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

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