Hexobarbital M (OH, -H2O)

Inchi: InChI=1S/C11H12N2O3/c1-11(7-5-3-2-4-6-7)8(14)12-10(16)13-9(11)15/h2-3,5H,4,6H2,1
InchiKey: ZQVVGVBZKRIZQO-UHFFFAOYSA-N
Formula: C11H12N2O3
SMILES: CC1(C2=CC=CCC2)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 220.22

Physical Properties

Property code	Value	Unit	Source
gf	-49.20	kJ/mol	Joback Method
hf	-359.54	kJ/mol	Joback Method
hfus	20.31	kJ/mol	Joback Method
hvap	67.60	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	0.635		Crippen Method
mcvol	160.200	ml/mol	McGowan Method
pc	4036.37	kPa	Joback Method
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook
tb	798.95	K	Joback Method
tc	1093.99	K	Joback Method
tf	685.39	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.83	J/mol×K	798.95	Joback Method
cpg	503.18	J/mol×K	848.12	Joback Method
cpg	520.24	J/mol×K	897.30	Joback Method
cpg	536.04	J/mol×K	946.47	Joback Method
cpg	550.61	J/mol×K	995.64	Joback Method
cpg	563.97	J/mol×K	1044.81	Joback Method
cpg	576.17	J/mol×K	1093.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R57505&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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