Heptabarbital M (OH, -H2O)

Inchi: InChI=1S/C13H16N2O3/c1-2-13(9-7-5-3-4-6-8-9)10(16)14-12(18)15-11(13)17/h5,7-8H,2-

InchiKey: IYKIYSHDMFBWDO-UHFFFAOYSA-N

Formula: C13H16N2O3

SMILES: CCC1(C2=CCCCC=C2)C(=O)NC(=O)NC1=O

Mol. weight [g/mol]: 248.28

Physical Properties

Property code	Value	Unit	Source
gf	-44.46	kJ/mol	Joback Method
hf	-406.98	kJ/mol	Joback Method
hfus	23.39	kJ/mol	Joback Method
hvap	72.22	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	1.415		Crippen Method
mcvol	188.380	ml/mol	McGowan Method
pc	3299.15	kPa	Joback Method
rinpol	2300.00		NIST Webbook
tb	848.98	K	Joback Method
tc	1137.32	K	Joback Method
tf	704.41	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.00	J/mol×K	848.98	Joback Method
cpg	620.43	J/mol×K	897.04	Joback Method
cpg	638.29	J/mol×K	945.09	Joback Method
cpg	654.60	J/mol×K	993.15	Joback Method
cpg	669.39	J/mol×K	1041.21	Joback Method
cpg	682.69	J/mol×K	1089.26	Joback Method
cpg	694.53	J/mol×K	1137.32	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=R493557&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