Cyclobarbital M (OH, -H2O)

Inchi: InChI=1S/C12H14N2O3/c1-2-12(8-6-4-3-5-7-8)9(15)13-11(17)14-10(12)16/h3-4,6H,2,5,7
InchiKey: QYYZSKOKTPFFLD-UHFFFAOYSA-N
Formula: C12H14N2O3
SMILES: CCC1(C2=CC=CCC2)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 234.25

Physical Properties

Property code	Value	Unit	Source
gf	-40.78	kJ/mol	Joback Method
hf	-380.18	kJ/mol	Joback Method
hfus	22.90	kJ/mol	Joback Method
hvap	69.82	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	1.025		Crippen Method
mcvol	174.290	ml/mol	McGowan Method
pc	3585.64	kPa	Joback Method
rinpol	2170.00		NIST Webbook
tb	821.83	K	Joback Method
tc	1108.98	K	Joback Method
tf	696.66	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.56	J/mol×K	821.83	Joback Method
cpg	559.21	J/mol×K	869.69	Joback Method
cpg	576.55	J/mol×K	917.55	Joback Method
cpg	592.60	J/mol×K	965.40	Joback Method
cpg	607.41	J/mol×K	1013.26	Joback Method
cpg	621.01	J/mol×K	1061.12	Joback Method
cpg	633.44	J/mol×K	1108.98	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R57395&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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