Cyclopentobarbital

Other names:	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(2-cyclopenten-1-yl)-5-(2-propenyl)-
	Barbituric acid, 5-allyl-5-(2-cyclopentenyl)-
	Allylcyclopentenylbarbital
	5-Allyl-5-(2-cyclopentenyl)barbituric acid
	Allylpental
	Ciclopal
	Cyclopal
	Cyclopen
	Cyclopental
	Cyclopentenyl allylbarbituric acid
	Dormisan
	Cyclopentobarbitone
	5-(2-Cyclopenten-1-yl)-5-(2-propenyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
	5-Allyl-5-(2-cyclopenten-1-yl)barbituric acid
	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(2-cyclopenten-1-yl)-5-(2-propen-1-yl)-
	Allylcyclopentenylbarbituric acid
	5-Allyl-5-(2-cyclopenten-1-yl)-2,4,6(1H,3H,5H)-pyrimidinetrione
Inchi:	InChI=1S/C12H14N2O3/c1-2-7-12(8-5-3-4-6-8)9(15)13-11(17)14-10(12)16/h2-3,5,8H,1,4
InchiKey:	XOVJAYNMQDTIJD-UHFFFAOYSA-N
Formula:	C12H14N2O3
SMILES:	C=CCC1(C2C=CCC2)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	234.25
CAS:	76-68-6

Physical Properties

Property code	Value	Unit	Source
gf	31.12	kJ/mol	Joback Method
hf	-315.24	kJ/mol	Joback Method
hfus	23.96	kJ/mol	Joback Method
hvap	67.72	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	0.881		Crippen Method
mcvol	174.290	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	1868.00		NIST Webbook
rinpol	1862.00		NIST Webbook
rinpol	1862.00		NIST Webbook

rinpol	1858.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1868.00		NIST Webbook
rinpol	1858.00		NIST Webbook
tb	805.43	K	Joback Method
tc	1087.01	K	Joback Method
tf	680.90	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.17	J/mol×K	805.43	Joback Method
cpg	562.18	J/mol×K	852.36	Joback Method
cpg	579.95	J/mol×K	899.29	Joback Method
cpg	596.52	J/mol×K	946.22	Joback Method
cpg	611.98	J/mol×K	993.15	Joback Method
cpg	626.36	J/mol×K	1040.08	Joback Method
cpg	639.73	J/mol×K	1087.01	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C76686&Units=SI

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