Heptabarbital

Other names:	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-cyclohepten-1-yl)-5-ethyl-
	5-(1-Cyclohepten-1-Yl)-5-ethyl-2,4,6(1H,3H,5H)-pyrimidinetrione
	5-(1-Cyclohepten-1-yl)-5-ethylbarbituric acid
	5-(1-cycloheptenyl)-5-ethyl-1,3-diazinane-2,4,6-trione
	5-(Cyclohepten-1-yl)-5-ethylbarbituric acid
	5-Ethyl-5-(1'-cycloheptenyl)-barbituric acid
	5-Ethyl-5-cycloheptenylbarbituric acid
	Barbituric acid, 5-(1-cyclohepten-1-yl)-5-ethyl-
	Cycloheptenylethylbarbituric acid
	Cycloheptenylethylmalonylurea
	G 475
	Heptabarb
	Heptabarbitone
	Heptabarbum
	Heptadorm
	Heptamal
	Heptbarbital
	Medapan
	Medomin
	Medomine
	Noctyn
Inchi:	InChI=1S/C13H18N2O3/c1-2-13(9-7-5-3-4-6-8-9)10(16)14-12(18)15-11(13)17/h7H,2-6,8
InchiKey:	PAZQYDJGLKSCSI-UHFFFAOYSA-N
Formula:	C13H18N2O3
SMILES:	CCC1(C2=CCCCCC2)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	250.29
CAS:	509-86-4

Physical Properties

Property code	Value	Unit	Source
gf	-74.42	kJ/mol	Joback Method
hf	-464.76	kJ/mol	Joback Method
hfus	22.17	kJ/mol	Joback Method
hvap	71.93	kJ/mol	Joback Method
log10ws	-3.00		Aqueous Solubility Prediction Method
logp	1.639		Crippen Method

mcvol	192.680	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	2045.00		NIST Webbook
rinpol	2036.00		NIST Webbook
rinpol	2090.00		NIST Webbook
rinpol	2075.00		NIST Webbook
rinpol	2067.00		NIST Webbook
rinpol	2035.00		NIST Webbook
rinpol	2098.00		NIST Webbook
rinpol	2058.00		NIST Webbook
rinpol	2065.00		NIST Webbook
rinpol	2098.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
rinpol	2041.00		NIST Webbook
rinpol	2047.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2067.00		NIST Webbook
rinpol	2036.00		NIST Webbook
rinpol	2098.00		NIST Webbook
tb	849.82	K	Joback Method
tc	1135.56	K	Joback Method
tf	447.35	K	Aqueous Solubility Prediction Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.40	J/mol×K	849.82	Joback Method
cpg	649.78	J/mol×K	897.44	Joback Method
cpg	668.51	J/mol×K	945.07	Joback Method
cpg	685.62	J/mol×K	992.69	Joback Method
cpg	701.12	J/mol×K	1040.31	Joback Method
cpg	715.03	J/mol×K	1087.94	Joback Method
cpg	727.38	J/mol×K	1135.56	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C509864&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