Barbital

Other names:	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5,5-diethyl-
	5,5-Diethyl-2,4,6(1H,3H,5H)-pyrimidinetrione
	5,5-Diethylbarbituric acid
	Barbitone
	Barbituric acid, 5,5-diethyl-
	Deba
	Diemal
	Diethylbarbitone
	Diethylbarbituric acid
	Diethylmalonylurea
	Dormonal
	Ethylbarbital
	Hypnogene
	Kyselina 5,5-diethylbarbiturova
	Malonal
	Metharbital M (nor)
	NSC 31352
	Sedeval
	Uronal
	Veroletten
	Verolettin
	Veronal
	Vesperal
Inchi:	InChI=1S/C8H12N2O3/c1-3-8(4-2)5(11)9-7(13)10-6(8)12/h3-4H2,1-2H3,(H2,9,10,11,12,1
InchiKey:	FTOAOBMCPZCFFF-UHFFFAOYSA-N
Formula:	C8H12N2O3
SMILES:	CCC1(CC)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	184.19
CAS:	57-44-3

Physical Properties

Property code	Value	Unit	Source
chs	-4127.50	kJ/mol	NIST Webbook
chs	-4126.00	kJ/mol	NIST Webbook
gf	-156.91	kJ/mol	Joback Method
hf	-476.37	kJ/mol	Joback Method

hfus	0.70	kJ/mol	Structural studies of cyclic ureas: 3. Enthalpy of formation of barbital
hsub	117.30 ± 0.60	kJ/mol	NIST Webbook
hvap	58.94	kJ/mol	Joback Method
log10ws	-1.41		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-2.40		Estimated Solubility Method
log10ws	-1.55		Aqueous Solubility Prediction Method
logp	0.159		Crippen Method
mcvol	137.390	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
rinpol	1536.90		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1480.00		NIST Webbook

rinpol	1480.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1461.00		NIST Webbook
tb	702.79	K	Joback Method
tc	967.84	K	Joback Method
tf	463.00 ± 4.00	K	NIST Webbook
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.82	J/mol×K	702.79	Joback Method
cpg	404.44	J/mol×K	746.96	Joback Method
cpg	420.27	J/mol×K	791.14	Joback Method
cpg	435.31	J/mol×K	835.31	Joback Method
cpg	449.56	J/mol×K	879.49	Joback Method
cpg	462.99	J/mol×K	923.66	Joback Method
cpg	475.62	J/mol×K	967.84	Joback Method
hfust	24.80	kJ/mol	462.00	NIST Webbook
hfust	24.98	kJ/mol	462.60	NIST Webbook
hsubt	113.90 ± 0.60	kJ/mol	366.00	NIST Webbook

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57443&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Structural studies of cyclic ureas: 3. Enthalpy of formation of barbital: https://www.doi.org/10.1016/j.jct.2009.06.018

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

chs:	Standard solid enthalpy of combustion
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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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