Butabarbital

Other names:	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(1-methylpropyl)-
	5-Ethyl-5-(1-methylpropyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
	5-Ethyl-5-(1-methylpropyl)barbituric acid
	5-Sec-butyl-5-ethyl-2,4,6(1H,3H,5H)-pyrimidinetrione
	5-sec-Butyl-5-Ethylbarbituric acid
	5-sec-Butyl-5-ethylmalonyl urea
	Barbituric acid, 5-sec-butyl-5-ethyl-
	Butabarb
	Butabarbitone
	Butatab
	Butatal
	Buticaps
	Butisol
	Butrate
	Medarsed
	NSC 27517
	Nilox
	Secbubarbital
	Secbutabarbital
	Secbutobarbital
	Secbutobarbitone
	Unicelles
	component of Pyridium plus
Inchi:	InChI=1S/C10H16N2O3/c1-4-6(3)10(5-2)7(13)11-9(15)12-8(10)14/h6H,4-5H2,1-3H3,(H2
InchiKey:	ZRIHAIZYIMGOAB-UHFFFAOYSA-N
Formula:	C10H16N2O3
SMILES:	CCC(C)C1(CC)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	212.25
CAS:	125-40-6

Physical Properties

Property code	Value	Unit	Source
gf	-142.51	kJ/mol	Joback Method
hf	-522.93	kJ/mol	Joback Method
hfus	21.38	kJ/mol	Joback Method
hvap	63.00	kJ/mol	Joback Method

log10ws	-2.39		Estimated Solubility Method
log10ws	-2.38		Aqueous Solubility Prediction Method
logp	0.795		Crippen Method
mcvol	165.570	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
rinpol	1634.00		NIST Webbook
rinpol	1701.10		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1634.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1703.40		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1680.00		NIST Webbook
tb	748.11	K	Joback Method
tc	1006.09	K	Joback Method
tf	439.65	K	Aqueous Solubility Prediction Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.00	J/mol×K	748.11	Joback Method
cpg	513.20	J/mol×K	791.11	Joback Method
cpg	530.43	J/mol×K	834.10	Joback Method
cpg	546.71	J/mol×K	877.10	Joback Method
cpg	562.04	J/mol×K	920.10	Joback Method
cpg	576.42	J/mol×K	963.09	Joback Method

cpg	589.86	J/mol×K	1006.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C125406&Units=SI
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
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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