Butethal

Other names:	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-butyl-5-ethyl-
	5-Butyl-5-ethyl-2,4,6(1H,3H,5H)-pyrimidinetrione
	5-Butyl-5-ethylbarbituric acid
	5-Ethyl-5-butylbarbituric acid
	5-Ethyl-5-n-butylbarbituric acid
	5-butyl-5-ethyl-1,3-diazinane-2,4,6-trione
	Barbituric acid, 5-butyl-5-ethyl-
	Budorm
	Butabarbitol
	Butobarbital
	Butobarbitone
	Butobarbitural
	Butyl,5-ethylbarbituric acid
	Etoval
	Hyperbutal
	Longanoct
	Meonal
	Monodorm
	NSC 229336
	Neonal
	Sonerile
	Soneryl
Inchi:	InChI=1S/C10H16N2O3/c1-3-5-6-10(4-2)7(13)11-9(15)12-8(10)14/h3-6H2,1-2H3,(H2,11,
InchiKey:	STDBAQMTJLUMFW-UHFFFAOYSA-N
Formula:	C10H16N2O3
SMILES:	CCCCC1(CC)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	212.25
CAS:	77-28-1

Physical Properties

Property code	Value	Unit	Source
gf	-140.07	kJ/mol	Joback Method
hf	-517.65	kJ/mol	Joback Method
hfus	24.90	kJ/mol	Joback Method
hvap	63.39	kJ/mol	Joback Method

log10ws	-1.69		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-1.66		Aqueous Solubility Prediction Method
log10ws	-1.66		Estimated Solubility Method
logp	0.939		Crippen Method
mcvol	165.570	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
rinpol	1702.90		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1642.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1641.00		NIST Webbook
rinpol	1641.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1642.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1642.00		NIST Webbook
tb	748.55	K	Joback Method
tc	1001.43	K	Joback Method
tf	400.90	K	Aqueous Solubility Prediction Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.44	J/mol×K	748.55	Joback Method
cpg	512.28	J/mol×K	790.70	Joback Method

cpg	529.20	J/mol×K	832.84	Joback Method
cpg	545.22	J/mol×K	874.99	Joback Method
cpg	560.34	J/mol×K	917.14	Joback Method
cpg	574.57	J/mol×K	959.29	Joback Method
cpg	587.91	J/mol×K	1001.43	Joback Method

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=C77281&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

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