Butalbital

Other names: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(2-methylpropyl)-5-(2-propenyl)-
5-(2-methylpropyl)-5-prop-2-enyl-1,3-diazinane-2,4,6-trione
5-Allyl-5-(2'-methyl-n-propyl) barbituric acid
5-Allyl-5-(2-methylpropyl)barbituric acid
5-Allyl-5-isobutyl-2,4,6(1H,3H,5H)-pyrimidinetrione
5-Allyl-5-isobutylbarbituric acid
Alisobumal
Allylbarbital
Allylbarbitone
Allylbarbituric acid
Allylisobutylbarbital
Allylisobutylbarbituric acid
Barbituric acid, 5-allyl-5-isobutyl-
Butalbarbital
Isobutylallylbarbituric acid
Isobutylallylbarturic acid
Itobarbital
Optalidon
Profundal
Sandoptal
Tetrallobarbital

Inchi: InChI=1S/C11H16N2O3/c1-4-5-11(6-7(2)3)8(14)12-10(16)13-9(11)15/h4,7H,1,5-6H2,2-3

InchiKey: UZVHFVZFNXBMQJ-UHFFFAOYSA-N

Formula: C11H16N2O3

SMILES: C=CCC1(CC(C)C)C(=O)NC(=O)NC1=O

Mol. weight [g/mol]: 224.26

CAS: 77-26-9

Physical Properties

Property code	Value	Unit	Source
gf	-46.25	kJ/mol	Joback Method
hf	-418.14	kJ/mol	Joback Method
hfus	22.69	kJ/mol	Joback Method
hvap	64.56	kJ/mol	Joback Method
log10ws	-2.12		Aqueous Solubility Prediction Method

log10ws	-2.12		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.961		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	1637.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1704.50		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1634.00		NIST Webbook
rinpol	1694.00		NIST Webbook
rinpol	1684.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1706.10		NIST Webbook
rinpol	1642.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1643.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1684.00		NIST Webbook
rinpol	1642.00		NIST Webbook
rinpol	1684.00		NIST Webbook
tb	767.67	K	Joback Method
tc	1025.00	K	Joback Method
tf	411.75	K	Aqueous Solubility Prediction Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.76	J/mol×K	767.67	Joback Method
cpg	542.80	J/mol×K	810.56	Joback Method
cpg	559.87	J/mol×K	853.45	Joback Method
cpg	575.99	J/mol×K	896.34	Joback Method
cpg	591.16	J/mol×K	939.22	Joback Method
cpg	605.41	J/mol×K	982.11	Joback Method
cpg	618.77	J/mol×K	1025.00	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
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=C77269&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