

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-methylbutyl)-5-(2-propenyl)-

Other names: (.+/-.)-Secobarbital
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-methylbutyl)-5-(2-propen-1-yl)-
2,4,6(1H,3H,5H)-Pyrimidinitrione, 5-(1-methylbutyl)-5-(2-propenyl)-
5-(1-Methylbutyl)-5-(2-propen-1-yl)-2,4,6(1H,3H,5H)-pyrimidinetrione (secobarbital)
5-Allyl-5-(1-methylbutyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
5-Allyl-5-(1-methylbutyl)barbituric acid
5-Allyl-5-(1-methylbutyl)malonylurea
5-pentan-2-yl-5-prop-2-enyl-1,3-diazinane-2,4,6-trione
Barbituric acid, 5-allyl-5-(1-methylbutyl)-
Barbosec
Evronal
Hypotrol
Immenox
Meballymal
Quinalbarbital
Quinalbarbitone
Secobarbital
Secobarbitone
Seconal

Inchi: InChI=1S/C12H18N2O3/c1-4-6-8(3)12(7-5-2)9(15)13-11(17)14-10(12)16/h5,8H,2,4,6-7H

InchiKey: KQPKPCNLIDLUMF-UHFFFAOYSA-N

Formula: C12H18N2O3

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

Mol. weight [g/mol]: 238.29

Physical Properties

Property code	Value	Unit	Source
hfus	25.28	kJ/mol	Joback Method
log10ws	-2.36		Aqueous Solubility Prediction Method
log10ws	-2.36		Estimated Solubility Method
logp	1.351		Crippen Method
mcvol	189.450	ml/mol	McGowan Method
rinpol	1813.00		NIST Webbook
rinpol	1831.30		NIST Webbook
rinpol	1795.00		NIST Webbook

rinpol	1810.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1777.00		NIST Webbook
rinpol	1786.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1795.00		NIST Webbook
rinpol	1815.00		NIST Webbook
rinpol	1795.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1791.00		NIST Webbook
rinpol	1769.00		NIST Webbook
rinpol	1763.00		NIST Webbook
rinpol	1810.00		NIST Webbook
rinpol	1769.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1763.00		NIST Webbook
rinpol	1768.00		NIST Webbook
rinpol	1757.00		NIST Webbook
rinpol	1766.00		NIST Webbook
rinpol	1769.00		NIST Webbook
rinpol	1763.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1788.00		NIST Webbook
rinpol	1788.00		NIST Webbook
rinpol	1763.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1786.00		NIST Webbook
rinpol	1791.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1831.30		NIST Webbook
rinpol	1769.00		NIST Webbook
rinpol	1763.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1775.00		NIST Webbook
tf	370.65	K	Aqueous Solubility Prediction Method
tf	356.70 ± 2.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.58	J/mol×K	790.55	Joback Method
cpg	599.01	J/mol×K	832.52	Joback Method
cpg	616.42	J/mol×K	874.48	Joback Method
cpg	632.84	J/mol×K	916.45	Joback Method
cpg	648.30	J/mol×K	958.41	Joback Method
cpg	662.81	J/mol×K	1000.38	Joback Method
cpg	676.40	J/mol×K	1042.34	Joback Method
hfust	22.90	kJ/mol	371.80	NIST Webbook

Sources

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C76733&Units=SI>

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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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