Secobarbital

Other names:	(.+/-.))-Secobarbital
	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-methylbutyl)-5-(2-propen-1-yl)-
	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-methylbutyl)-5-(2-propenyl)-
	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
	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]:	238.28
CAS:	76-73-3

Physical Properties

Property code	Value	Unit	Source
gf	-37.83	kJ/mol	Joback Method
hf	-438.78	kJ/mol	Joback Method
hfus	25.28	kJ/mol	Joback Method
hvap	66.78	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
pc	2726.86	kPa	Joback Method
rinpol	1763.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1769.00		NIST Webbook
rinpol	1810.00		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	1790.00		NIST Webbook
rinpol	1795.00		NIST Webbook
rinpol	1815.00		NIST Webbook
rinpol	1795.00		NIST Webbook
rinpol	1768.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1831.30		NIST Webbook
rinpol	1791.00		NIST Webbook
rinpol	1769.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1813.00		NIST Webbook
rinpol	1769.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1763.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1770.00		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	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	1795.00		NIST Webbook
rinpol	1763.00		NIST Webbook

rinpol	1775.00		NIST Webbook
rinpol	1831.30		NIST Webbook
rinpol	1820.00		NIST Webbook
tb	790.55	K	Joback Method
tc	1042.34	K	Joback Method
tf	356.70 ± 2.00	K	NIST Webbook
tf	370.65	K	Aqueous Solubility Prediction Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.81	J/mol×K	1000.38	Joback Method
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	676.40	J/mol×K	1042.34	Joback Method
hfust	22.90	kJ/mol	371.80	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C76733&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust:	Enthalpy of fusion 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