Dipropylbarbital

Other names:	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5,5-dipropyl-
	5,5-Dipropyl-2,4,6(1H,3H,5H)-pyrimidinetrione
	5,5-Dipropylbarbituric acid
	5,5-dipropyl-1,3-diazinane-2,4,6-trione
	Dipropylbarbituric acid
	Proponal
	Propylbarbital
	di-n-Propylbarbituric acid
Inchi:	InChI=1S/C10H16N2O3/c1-3-5-10(6-4-2)7(13)11-9(15)12-8(10)14/h3-6H2,1-2H3,(H2,11,
InchiKey:	RCOUWKSZRXJXLA-UHFFFAOYSA-N
Formula:	C10H16N2O3
SMILES:	CCCC1(CCC)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	212.25

Physical Properties

Property code	Value	Unit	Source
hfus	24.90	kJ/mol	Joback Method
ie	9.48	eV	Cheméo Relay (1.0)
log10ws	-2.53		Aqueous Solubility Prediction Method
log10ws	-2.53		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.939		Crippen Method
mcvol	165.570	ml/mol	McGowan Method
rinpol	1650.00		NIST Webbook
rinpol	1650.00		NIST Webbook
tf	456.05	K	Cheméo Relay (1.0)

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

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/AqueousDa
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2217085&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
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