Barbituric acid, 5,5-dipropyl-

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
	Dipropylbarbital
	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
CAS:	2217-08-5

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	-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
pc	3181.14	kPa	Joback Method
rinpol	1650.00		NIST Webbook
tb	748.55	K	Joback Method
tc	1001.43	K	Joback Method
tf	648.46	K	Joback 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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2217085&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

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

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