Barbituric acid, 5-allyl-5-neopentyl-

Other names:	Nealbarbital
	5-Allyl-5-neopentylbarbituric acid
	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(2,2-dimethylpropyl)-5-(2-propenyl)-
	Allylneopentylbarbituric acid
	Censedal
	Nealbarbitone
	Nepental
	Nevental
	5-Neopentyl-5-allylbarbituric acid
	5055
	5-(2,2-Dimethylpropyl)-5-(2-propenyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
	Neallymal
	5-Allyl-5-(2,2-dimethylpropyl)barbituric acid
Inchi:	InChI=1S/C12H18N2O3/c1-5-6-12(7-11(2,3)4)8(15)13-10(17)14-9(12)16/h5H,1,6-7H2,2-
InchiKey:	YHKPTICJRUESOY-UHFFFAOYSA-N
Formula:	C12H18N2O3
SMILES:	C=CCC1(CC(C)(C)C)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	238.28
CAS:	561-83-1

Physical Properties

Property code	Value	Unit	Source
gf	-32.55	kJ/mol	Joback Method
hf	-442.25	kJ/mol	Joback Method
hfus	21.39	kJ/mol	Joback Method
hvap	65.88	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	1.351		Crippen Method
mcvol	189.450	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
rinpol	1720.00		NIST Webbook
rinpol	1720.00		NIST Webbook
tb	787.76	K	Joback Method
tc	1048.64	K	Joback Method
tf	671.66	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.76	J/mol×K	787.76	Joback Method
cpg	600.44	J/mol×K	831.24	Joback Method
cpg	618.07	J/mol×K	874.72	Joback Method
cpg	634.73	J/mol×K	918.20	Joback Method
cpg	650.46	J/mol×K	961.68	Joback Method
cpg	665.33	J/mol×K	1005.16	Joback Method
cpg	679.41	J/mol×K	1048.64	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C561831&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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