Barbituric acid, 5-allyl-

Other names: 5-allylbarbituric acid
Inchi: InChI=1S/C7H8N2O3/c1-2-3-4-5(10)8-7(12)9-6(4)11/h2,4H,1,3H2,(H2,8,9,10,11,12)
InchiKey: JLXDSDWQIIJSHV-UHFFFAOYSA-N
Formula: C7H8N2O3
SMILES: C=CCC1C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 168.15
CAS: 2565-43-7

Physical Properties

Property code	Value	Unit	Source
gf	-72.00	kJ/mol	Joback Method
hf	-345.54	kJ/mol	Joback Method
hfus	22.15	kJ/mol	Joback Method
hvap	57.19	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	-0.455		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
pc	4516.42	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1660.00		NIST Webbook
tb	676.35	K	Joback Method
tc	943.37	K	Joback Method
tf	588.99	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.72	J/mol×K	676.35	Joback Method
cpg	332.83	J/mol×K	720.85	Joback Method
cpg	346.88	J/mol×K	765.36	Joback Method
cpg	359.70	J/mol×K	809.86	Joback Method
cpg	371.13	J/mol×K	854.36	Joback Method
cpg	381.02	J/mol×K	898.87	Joback Method

cpg	389.19	J/mol×K	943.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2565437&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
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