5-Allyl-5-(2-hydroxypropyl)barbituric acid

Inchi: InChI=1S/C12H16O4/c1-3-4-12(7-8(2)13)10(15)5-9(14)6-11(12)16/h3,8,13H,1,4-7H2,2H
InchiKey: KJXFGGZCXNUGME-UHFFFAOYSA-N
Formula: C12H16O4
SMILES: C=CCC1(CC(C)O)C(=O)CC(=O)CC1=O
Mol. weight [g/mol]: 224.25

Physical Properties

Property code	Value	Unit	Source
gf	-350.07	kJ/mol	Joback Method
hf	-666.63	kJ/mol	Joback Method
hfus	10.19	kJ/mol	Joback Method
hvap	69.95	kJ/mol	Joback Method
log10ws	-1.57		Crippen Method
logp	0.821		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
rinpol	1837.00		NIST Webbook
rinpol	1837.00		NIST Webbook
tb	785.63	K	Joback Method
tc	1014.81	K	Joback Method
tf	505.00	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.64	J/mol×K	785.63	Joback Method
cpg	556.18	J/mol×K	823.83	Joback Method
cpg	570.97	J/mol×K	862.02	Joback Method
cpg	585.07	J/mol×K	900.22	Joback Method
cpg	598.51	J/mol×K	938.42	Joback Method
cpg	611.34	J/mol×K	976.61	Joback Method
cpg	623.60	J/mol×K	1014.81	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=R536773&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