5-Vanillylidene barbituric acid

Inchi: InChI=1S/C12H10N2O5/c1-19-9-5-6(2-3-8(9)15)4-7-10(16)13-12(18)14-11(7)17/h2-5,15H
InchiKey: HOHGWOUABYDGBN-UHFFFAOYSA-N
Formula: C12H10N2O5
SMILES: COc1cc(C=C2C(O)=NC(=O)N=C2O)ccc1O
Mol. weight [g/mol]: 262.22
CAS: 40367-32-6

Physical Properties

Property code	Value	Unit	Source
gf	-151.07	kJ/mol	Joback Method
hf	-432.39	kJ/mol	Joback Method
hfus	38.17	kJ/mol	Joback Method
hvap	114.13	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.831		Crippen Method
mcvol	177.430	ml/mol	McGowan Method
pc	5160.85	kPa	Joback Method
tb	1007.38	K	Joback Method
tc	1252.10	K	Joback Method
tf	779.37	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.59	J/mol×K	1007.38	Joback Method
cpg	587.10	J/mol×K	1048.17	Joback Method
cpg	592.36	J/mol×K	1088.95	Joback Method
cpg	596.38	J/mol×K	1129.74	Joback Method
cpg	599.15	J/mol×K	1170.53	Joback Method
cpg	600.66	J/mol×K	1211.31	Joback Method
cpg	600.91	J/mol×K	1252.10	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40367326&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume