5-Piperonylidenebarbituric acid

Inchi: InChI=1S/C12H8N2O5/c15-10-7(11(16)14-12(17)13-10)3-6-1-2-8-9(4-6)19-5-18-8/h1-4H
InchiKey: NSJGTQPGBBWIIQ-UHFFFAOYSA-N
Formula: C12H8N2O5
SMILES: O=C1N=C(O)C(=Cc2ccc3c(c2)OCO3)C(O)=N1
Mol. weight [g/mol]: 260.20
CAS: 4551-03-5

Physical Properties

Property code	Value	Unit	Source
gf	-4.86	kJ/mol	Joback Method
hf	-305.19	kJ/mol	Joback Method
hfus	43.84	kJ/mol	Joback Method
hvap	108.61	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	1.845		Crippen Method
mcvol	166.570	ml/mol	McGowan Method
pc	5146.06	kPa	Joback Method
tb	974.63	K	Joback Method
tc	1220.87	K	Joback Method
tf	733.26	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.37	J/mol×K	974.63	Joback Method
cpg	549.71	J/mol×K	1015.67	Joback Method
cpg	554.74	J/mol×K	1056.71	Joback Method
cpg	558.47	J/mol×K	1097.75	Joback Method
cpg	560.89	J/mol×K	1138.79	Joback Method
cpg	562.00	J/mol×K	1179.83	Joback Method
cpg	561.81	J/mol×K	1220.87	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=C4551035&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