1,3-Dinitrophenoxazine

Inchi: InChI=1S/C12H7N3O5/c16-14(17)7-5-9(15(18)19)12-11(6-7)20-10-4-2-1-3-8(10)13-12/h
InchiKey: BNCNPPGADFFASS-UHFFFAOYSA-N
Formula: C12H7N3O5
SMILES: O=[N+]([O-])c1cc2c(c([N+](=O)[O-])c1)Nc1ccccc1O2
Mol. weight [g/mol]: 273.20
CAS: 26103-32-2

Physical Properties

Property code	Value	Unit	Source
gf	389.71	kJ/mol	Joback Method
hf	119.76	kJ/mol	Joback Method
hfus	52.82	kJ/mol	Joback Method
hvap	94.01	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.352		Crippen Method
mcvol	172.250	ml/mol	McGowan Method
pc	3955.54	kPa	Joback Method
tb	933.56	K	Joback Method
tc	1227.57	K	Joback Method
tf	772.44	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.36	J/mol×K	933.56	Joback Method
cpg	500.58	J/mol×K	982.56	Joback Method
cpg	509.21	J/mol×K	1031.56	Joback Method
cpg	517.40	J/mol×K	1080.56	Joback Method
cpg	525.33	J/mol×K	1129.57	Joback Method
cpg	533.17	J/mol×K	1178.57	Joback Method
cpg	541.08	J/mol×K	1227.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26103322&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

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