3-Methoxy-5-nitrosalicylaldehyde

Other names:	2-Hydroxy-3-methoxy-5-nitrobenzaldehyde
	Benzaldehyde, 2-hydroxy-3-methoxy-5-nitro-
Inchi:	InChI=1S/C8H7NO5/c1-14-7-3-6(9(12)13)2-5(4-10)8(7)11/h2-4,11H,1H3
InchiKey:	HGKHVFKBOHFYSS-UHFFFAOYSA-N
Formula:	C8H7NO5
SMILES:	COc1cc([N+](=O)[O-])cc(C=O)c1O
Mol. weight [g/mol]:	197.14
CAS:	17028-61-4

Physical Properties

Property code	Value	Unit	Source
gf	-213.96	kJ/mol	Joback Method
hf	-400.73	kJ/mol	Joback Method
hfus	30.36	kJ/mol	Joback Method
hvap	75.74	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.121		Crippen Method
mcvol	130.550	ml/mol	McGowan Method
pc	4646.65	kPa	Joback Method
tb	722.62	K	Joback Method
tc	973.09	K	Joback Method
tf	550.94	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.61	J/mol×K	722.62	Joback Method
cpg	345.30	J/mol×K	764.36	Joback Method
cpg	353.42	J/mol×K	806.11	Joback Method
cpg	361.01	J/mol×K	847.85	Joback Method
cpg	368.15	J/mol×K	889.60	Joback Method
cpg	374.91	J/mol×K	931.34	Joback Method
cpg	381.36	J/mol×K	973.09	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=C17028614&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