BENZALDEHYDE, 2-HYDROXY-3-METHOXY-5-NITRO-

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]: 197.15

Physical Properties

Property code	Value	Unit	Source
hfus	30.36	kJ/mol	Joback Method
ie	9.20	eV	Cheméo Relay (1.0)
log10ws	-1.95		Cheméo Relay (1.0)
logp	1.122		Crippen Method
mcvol	130.550	ml/mol	McGowan Method
tb	564.05	K	Cheméo Relay (1.0)
tf	386.69	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17028614&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point