3-Methoxy-2-nitrobenzoic acid

Other names: 2-Nitro-3-methoxybenzoic acid
Benzoic acid, 3-methoxy-2-nitro-
m-Anisic acid, 2-nitro-
Inchi: InChI=1S/C8H7NO5/c1-14-6-4-2-3-5(8(10)11)7(6)9(12)13/h2-4H,1H3,(H,10,11)
InchiKey: YMOMYSDAOXOCID-UHFFFAOYSA-N
Formula: C8H7NO5
SMILES: COc1cccc(C(=O)O)c1[N+](=O)[O-]
Mol. weight [g/mol]: 197.14
CAS: 4920-80-3

Physical Properties

Property code	Value	Unit	Source
gf	-225.56	kJ/mol	Joback Method
hf	-402.65	kJ/mol	Joback Method
hfus	27.98	kJ/mol	Joback Method
hsub	141.90 ± 1.30	kJ/mol	NIST Webbook
hvap	79.43	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.302		Crippen Method
mcvol	130.550	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
tb	739.39	K	Joback Method
tc	966.92	K	Joback Method
tf	507.97	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.61	J/mol×K	739.39	Joback Method
cpg	344.79	J/mol×K	777.31	Joback Method
cpg	352.32	J/mol×K	815.23	Joback Method
cpg	359.20	J/mol×K	853.16	Joback Method
cpg	365.43	J/mol×K	891.08	Joback Method

cpg	371.04	J/mol×K	929.00	Joback Method
cpg	376.02	J/mol×K	966.92	Joback Method
hsubt	136.60 ± 1.30	kJ/mol	404.00	NIST Webbook

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=C4920803&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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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