3-METHOXY-4-NITROBENZOIC ACID

Other names: Benzoic acid, 3-methoxy-4-nitro-
Inchi: InChI=1S/C8H7NO5/c1-14-7-4-5(8(10)11)2-3-6(7)9(12)13/h2-4H,1H3,(H,10,11)
InchiKey: PWURRRRGLCVBMX-UHFFFAOYSA-N
Formula: C8H7NO5
SMILES: COc1cc(C(=O)O)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 197.15

Physical Properties

Property code	Value	Unit	Source
hf	-418.96	kJ/mol	Cheméo Relay (1.0)
hfus	27.98	kJ/mol	Joback Method
hsub	131.00 ± 1.10	kJ/mol	NIST Webbook
hvap	103.36	kJ/mol	Cheméo Relay (1.0)
ie	9.36	eV	Cheméo Relay (1.0)
log10ws	-2.57		Cheméo Relay (1.0)
logp	1.302		Crippen Method
mcvol	130.550	ml/mol	McGowan Method
tb	571.44	K	Cheméo Relay (1.0)
tf	399.32	K	Cheméo Relay (1.0)

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	126.10 ± 1.10	kJ/mol	395.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5081367&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

Legend

cpg:	Ideal gas heat capacity
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
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