methyl 4-hydroxy-3-nitrobenzoate

Inchi: InChI=1S/C8H7NO5/c1-14-8(11)5-2-3-7(10)6(4-5)9(12)13/h2-4,10H,1H3
InchiKey: GNCWCTBHZCBXGL-UHFFFAOYSA-N
Formula: C8H7NO5
SMILES: COC(=O)c1ccc(O)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 197.14
CAS: 99-42-3

Physical Properties

Property code	Value	Unit	Source
gf	-233.73	kJ/mol	Joback Method
hf	-416.26	kJ/mol	Joback Method
hfus	30.06	kJ/mol	Joback Method
hvap	75.10	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.087		Crippen Method
mcvol	130.550	ml/mol	McGowan Method
pc	4672.09	kPa	Joback Method
tb	722.85	K	Joback Method
tc	977.75	K	Joback Method
tf	546.35	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.39	J/mol×K	722.85	Joback Method
cpg	346.42	J/mol×K	765.33	Joback Method
cpg	354.80	J/mol×K	807.82	Joback Method
cpg	362.60	J/mol×K	850.30	Joback Method
cpg	369.90	J/mol×K	892.78	Joback Method
cpg	376.79	J/mol×K	935.27	Joback Method
cpg	383.34	J/mol×K	977.75	Joback Method

Sources

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=C99423&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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