Ethyl 4-hydroxy-3-nitrobenzoate

Other names: Benzoic acid, 4-hydroxy-3-nitro-, ethyl ester
Inchi: InChI=1S/C9H9NO5/c1-2-15-9(12)6-3-4-8(11)7(5-6)10(13)14/h3-5,11H,2H2,1H3
InchiKey: FBHJNBWUGONVNS-UHFFFAOYSA-N
Formula: C9H9NO5
SMILES: CCOC(=O)c1ccc(O)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 211.17
CAS: 19013-10-6

Physical Properties

Property code	Value	Unit	Source
gf	-225.31	kJ/mol	Joback Method
hf	-436.90	kJ/mol	Joback Method
hfus	32.65	kJ/mol	Joback Method
hvap	77.33	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	1.477		Crippen Method
mcvol	144.640	ml/mol	McGowan Method
pc	4114.41	kPa	Joback Method
tb	745.73	K	Joback Method
tc	995.02	K	Joback Method
tf	557.62	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.96	J/mol×K	745.73	Joback Method
cpg	396.80	J/mol×K	787.28	Joback Method
cpg	405.96	J/mol×K	828.83	Joback Method
cpg	414.52	J/mol×K	870.37	Joback Method
cpg	422.56	J/mol×K	911.92	Joback Method
cpg	430.16	J/mol×K	953.47	Joback Method
cpg	437.40	J/mol×K	995.02	Joback Method

Sources

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=C19013106&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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