Methyl 3-methoxy-4-nitrobenzoate

Other names:	Benzoic acid, 5-methoxy-4-nitro-, methyl(ester)
Inchi:	InChI=1S/C9H9NO5/c1-14-8-5-6(9(11)15-2)3-4-7(8)10(12)13/h3-5H,1-2H3
InchiKey:	PVVFEPFLFHDHHK-UHFFFAOYSA-N
Formula:	C9H9NO5
SMILES:	COC(=O)c1ccc([N+](=O)[O-])c(OC)c1
Mol. weight [g/mol]:	211.17
CAS:	5081-37-8

Physical Properties

Property code	Value	Unit	Source
gf	-185.32	kJ/mol	Joback Method
hf	-403.28	kJ/mol	Joback Method
hfus	27.67	kJ/mol	Joback Method
hvap	67.38	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	1.390		Crippen Method
mcvol	144.640	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	692.51	K	Joback Method
tc	931.93	K	Joback Method
tf	480.65	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.58	J/mol×K	692.51	Joback Method
cpg	378.70	J/mol×K	732.41	Joback Method
cpg	388.98	J/mol×K	772.32	Joback Method
cpg	398.43	J/mol×K	812.22	Joback Method
cpg	407.02	J/mol×K	852.12	Joback Method
cpg	414.76	J/mol×K	892.02	Joback Method
cpg	421.62	J/mol×K	931.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5081378&Units=SI
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

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

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