

Benzoic acid, 3-nitro-, methyl ester

Other names:	Benzoic acid, m-nitro-, methyl ester m-Nitrobenzoic acid, methyl ester Methyl m-nitrobenzoate Methyl 3-nitrobenzoate Methyl meta-nitrobenzoate 3-O ₂ N-C ₆ H ₄ -COOCH ₃
Inchi:	InChI=1S/C ₈ H ₇ NO ₄ /c1-13-8(10)6-3-2-4-7(5-6)9(11)12/h2-5H,1H3
InchiKey:	AXLYJLKKPUICKV-UHFFFAOYSA-N
Formula:	C ₈ H ₇ NO ₄
SMILES:	<chem>COC(=O)c1cccc([N+](=O)[O-])c1</chem>
Mol. weight [g/mol]:	181.15
CAS:	618-95-1

Physical Properties

Property code	Value	Unit	Source
affp	815.70	kJ/mol	NIST Webbook
basg	784.70	kJ/mol	NIST Webbook
ea	1.23 ± 0.09	eV	NIST Webbook
gf	-79.11	kJ/mol	Joback Method
hf	-238.95	kJ/mol	Joback Method
hfus	24.28	kJ/mol	Joback Method
hvap	62.09	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.381		Crippen Method
mcvol	124.680	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
tb	552.20	K	NIST Webbook
tc	889.97	K	Joback Method
tf	434.63	K	Joback Method
vc	0.481	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	298.26	J/mol×K	642.23	Joback Method
cpg	308.88	J/mol×K	683.52	Joback Method
cpg	318.68	J/mol×K	724.81	Joback Method
cpg	327.67	J/mol×K	766.10	Joback Method
cpg	335.88	J/mol×K	807.39	Joback Method
cpg	343.31	J/mol×K	848.68	Joback Method
cpg	349.99	J/mol×K	889.97	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=C618951&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
ea:	Electron affinity
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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