

Ethyl 3-nitrobenzoate

Other names:	Ethyl-m-nitrobenzoate Benzoic acid, 3-nitro-, ethyl ester m-Nitrobenzoic acid, ethyl ester Benzoic acid, m-nitro-, ethyl ester
Inchi:	InChI=1S/C9H9NO4/c1-2-14-9(11)7-4-3-5-8(6-7)10(12)13/h3-6H,2H2,1H3
InchiKey:	MKBIJCPQTPFQKQ-UHFFFAOYSA-N
Formula:	C9H9NO4
SMILES:	CCOC(=O)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	195.17
CAS:	618-98-4

Physical Properties

Property code	Value	Unit	Source
gf	-70.69	kJ/mol	Joback Method
hf	-259.59	kJ/mol	Joback Method
hfus	26.87	kJ/mol	Joback Method
hvap	64.31	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	1.771		Crippen Method
mcvol	138.770	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
tb	665.11	K	Joback Method
tc	907.46	K	Joback Method
tf	445.90	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.70	J/mol×K	867.07	Joback Method
cpg	345.96	J/mol×K	665.11	Joback Method
cpg	357.42	J/mol×K	705.50	Joback Method
cpg	367.99	J/mol×K	745.89	Joback Method
cpg	377.72	J/mol×K	786.28	Joback Method

cpg	386.61	J/mol×K	826.67	Joback Method
cpg	401.99	J/mol×K	907.46	Joback Method
hvapt	65.10	kJ/mol	476.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	429.20	K	1.30	NIST Webbook

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=C618984&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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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