Benzoic acid, 4-nitro-, ethyl ester

Other names:	Benzoic acid, p-nitro-, ethyl ester
	p-Nitrobenzoic acid, ethyl ester
	Ethyl nitrobenzoate, para ester
	Ethyl p-nitrobenzoate
	Ethyl 4-nitrobenzoate
	4-Nitrobenzoic acid ethyl ester
	Ethyl para-nitrobenzoate
	4-(Ethoxycarbonyl)nitrobenzene
	NSC 6763
Inchi:	InChI=1S/C9H9NO4/c1-2-14-9(11)7-3-5-8(6-4-7)10(12)13/h3-6H,2H2,1H3
InchiKey:	PHWSCBWNPZDYRI-UHFFFAOYSA-N
Formula:	C9H9NO4
SMILES:	CCOC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	195.17
CAS:	99-77-4

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
rinpol	1501.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1527.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1501.00		NIST Webbook

rinpol	1501.00		NIST Webbook
rinpol	1500.00		NIST Webbook
ripol	2334.00		NIST Webbook
ripol	2298.00		NIST Webbook
ripol	2280.00		NIST Webbook
ripol	2275.00		NIST Webbook
ripol	2280.00		NIST Webbook
ripol	2351.00		NIST Webbook
ripol	2326.00		NIST Webbook
ripol	2307.00		NIST Webbook
ripol	2343.00		NIST Webbook
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	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	394.70	J/mol×K	867.07	Joback Method
cpg	401.99	J/mol×K	907.46	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C99774&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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume