

AMINOFORMIC ACID, N-[3-NITROPHENYL]-, ETHYL(ESTER)

Other names:	Aminoformic acid, N-(3-nitrophenyl)-, ethyl ester Carbamic acid, 3-nitrophenyl, ethyl ester
Inchi:	InChI=1S/C9H10N2O4/c1-2-15-9(12)10-7-4-3-5-8(6-7)11(13)14/h3-6H,2H2,1H3,(H,10,12)
InchiKey:	JWPGACMNGJBXHB-UHFFFAOYSA-N
Formula:	C9H10N2O4
SMILES:	CCOC(=O)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	210.19

Physical Properties

Property code	Value	Unit	Source
hf	-326.49	kJ/mol	Cheméo Relay (1.0)
hfus	31.96	kJ/mol	Joback Method
hvap	93.56	kJ/mol	Cheméo Relay (1.0)
ie	8.92	eV	Cheméo Relay (1.0)
log10ws	-3.25		Cheméo Relay (1.0)
logp	2.163		Crippen Method
mcvol	148.750	ml/mol	McGowan Method
rinpol	1806.00		NIST Webbook
rinpol	1816.00		NIST Webbook
rinpol	1806.00		NIST Webbook
tb	578.67	K	Cheméo Relay (1.0)
tf	358.79	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.33	J/mol×K	715.28	Joback Method
cpg	403.45	J/mol×K	755.20	Joback Method
cpg	413.66	J/mol×K	795.11	Joback Method
cpg	423.00	J/mol×K	835.03	Joback Method
cpg	431.47	J/mol×K	874.95	Joback Method
cpg	439.11	J/mol×K	914.87	Joback Method
cpg	445.94	J/mol×K	954.78	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6275725&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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