

Carbamic acid, (2-nitrophenyl)-, ethyl ester

Other names:	Carbanilic acid, o-nitro-, ethyl ester 2-Nitrophenylurethane o-Nitro carbanilic acid, ethyl ester
Inchi:	InChI=1S/C9H10N2O4/c1-2-15-9(12)10-7-5-3-4-6-8(7)11(13)14/h3-6H,2H2,1H3,(H,10,12)
InchiKey:	AUDONQPVYRSJNX-UHFFFAOYSA-N
Formula:	C9H10N2O4
SMILES:	CCOC(=O)Nc1cccc1[N+](=O)[O-]
Mol. weight [g/mol]:	210.19
CAS:	2621-84-3

Physical Properties

Property code	Value	Unit	Source
gf	18.70	kJ/mol	Joback Method
hf	-206.12	kJ/mol	Joback Method
hfus	31.96	kJ/mol	Joback Method
hvap	70.75	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.163		Crippen Method
mcvol	148.750	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpol	1622.00		NIST Webbook
rinpol	1609.00		NIST Webbook
tb	715.28	K	Joback Method
tc	954.78	K	Joback Method
tf	498.56	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.33	J/molxK	715.28	Joback Method
cpg	403.45	J/molxK	755.20	Joback Method
cpg	413.66	J/molxK	795.11	Joback Method
cpg	423.00	J/molxK	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

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=C2621843&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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