

m-Nitro carbanilic acid, n-propyl ester

Other names:	Carbamic acid, 3-nitrophenyl-, propyl ester
Inchi:	InChI=1S/C10H12N2O4/c1-2-6-16-10(13)11-8-4-3-5-9(7-8)12(14)15/h3-5,7H,2,6H2,1H3,
InchiKey:	MQEORiyUQXEHOW-UHFFFAOYSA-N
Formula:	C10H12N2O4
SMILES:	CCCOC(=O)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	224.21
CAS:	91716-03-9

Physical Properties

Property code	Value	Unit	Source
gf	27.12	kJ/mol	Joback Method
hf	-226.76	kJ/mol	Joback Method
hfus	34.55	kJ/mol	Joback Method
hvap	72.98	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.553		Crippen Method
mcvol	162.840	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
tb	738.16	K	Joback Method
tc	973.02	K	Joback Method
tf	509.83	K	Joback Method
vc	0.628	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.18	J/mol×K	738.16	Joback Method
cpg	454.87	J/mol×K	777.30	Joback Method
cpg	465.63	J/mol×K	816.45	Joback Method
cpg	475.47	J/mol×K	855.59	Joback Method
cpg	484.42	J/mol×K	894.73	Joback Method
cpg	492.52	J/mol×K	933.88	Joback Method
cpg	499.78	J/mol×K	973.02	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=C91716039&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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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