

O-nitrocarbanilic acid, 3-hexen-1-ol ester

Inchi:	InChI=1S/C13H16N2O4/c1-2-3-4-7-10-19-13(16)14-11-8-5-6-9-12(11)15(17)18/h3-6,8-9
InchiKey:	ZWEYLUMVMZATIJ-ONEGZZNKSA-N
Formula:	C13H16N2O4
SMILES:	CCC=CCCOC(=O)Nc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	264.28
CAS:	92109-06-3

Physical Properties

Property code	Value	Unit	Source
gf	132.60	kJ/mol	Joback Method
hf	-171.46	kJ/mol	Joback Method
hfus	42.53	kJ/mol	Joback Method
hvap	79.61	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.500		Crippen Method
mcvol	200.810	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
tb	810.96	K	Joback Method
tc	1042.11	K	Joback Method
tf	538.56	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.49	J/molxK	810.96	Joback Method
cpg	588.88	J/molxK	849.48	Joback Method
cpg	600.30	J/molxK	888.01	Joback Method
cpg	610.80	J/molxK	926.53	Joback Method
cpg	620.45	J/molxK	965.06	Joback Method
cpg	629.29	J/molxK	1003.58	Joback Method
cpg	637.38	J/molxK	1042.11	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=C92109063&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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