

O-nitro carbanilic acid, nerol ester

Other names:	O-nitro carbanilic acid, geraniol ester
Inchi:	InChI=1S/C17H22N2O4/c1-13(2)7-6-8-14(3)11-12-23-17(20)18-15-9-4-5-10-16(15)19(21)
InchiKey:	GQRGGMFOGBGHJX-SDNWHVVSQSA-N
Formula:	C17H22N2O4
SMILES:	CC(C)=CCCC(C)=CCOC(=O)Nc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	318.37
CAS:	116373-28-5

Physical Properties

Property code	Value	Unit	Source
gf	229.40	kJ/mol	Joback Method
hf	-156.38	kJ/mol	Joback Method
hfus	50.47	kJ/mol	Joback Method
hvap	88.63	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	4.836		Crippen Method
mcvol	252.870	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
tb	906.40	K	Joback Method
tc	1138.96	K	Joback Method
tf	550.64	K	Joback Method
vc	0.983	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	772.67	J/mol×K	906.40	Joback Method
cpg	786.18	J/mol×K	945.16	Joback Method
cpg	798.77	J/mol×K	983.92	Joback Method
cpg	810.53	J/mol×K	1022.68	Joback Method
cpg	821.54	J/mol×K	1061.44	Joback Method
cpg	831.90	J/mol×K	1100.20	Joback Method
cpg	841.70	J/mol×K	1138.96	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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=C116373285&Units=SI

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
hvp:	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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