

O-nitro carbanilic acid, farnesol ester

Inchi:	InChI=1S/C22H30N2O4/c1-17(2)9-7-10-18(3)11-8-12-19(4)15-16-28-22(25)23-20-13-5-6
InchiKey:	RZEDEDGDSVTKGG-CFBAGHHKSA-N
Formula:	C22H30N2O4
SMILES:	CC(C)=CCCC(C)=CCCC(C)=CCOC(=O)Nc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	386.48
CAS:	100576-25-8

Physical Properties

Property code	Value	Unit	Source
gf	343.17	kJ/mol	Joback Method
hf	-152.15	kJ/mol	Joback Method
hfus	62.31	kJ/mol	Joback Method
hvap	99.80	kJ/mol	Joback Method
log10ws	-7.81		Crippen Method
logp	6.562		Crippen Method
mcvol	319.020	ml/mol	McGowan Method
pc	1301.41	kPa	Joback Method
tb	1024.84	K	Joback Method
tc	1261.92	K	Joback Method
tf	587.95	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1040.85	J/molxK	1024.84	Joback Method
cpg	1056.08	J/molxK	1064.35	Joback Method
cpg	1070.61	J/molxK	1103.87	Joback Method
cpg	1084.57	J/molxK	1143.38	Joback Method
cpg	1098.10	J/molxK	1182.89	Joback Method
cpg	1111.32	J/molxK	1222.41	Joback Method
cpg	1124.37	J/molxK	1261.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100576258&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	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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