

O-nitro carbanilic acid, santalol ester

Inchi:	InChI=1S/C22H28N2O4/c1-14(7-6-10-21(2)15-11-16-17(12-15)22(16,21)3)13-28-20(25)2
InchiKey:	BFPJUKRLKYMQDZ-AUWJEWJLSA-N
Formula:	C22H28N2O4
SMILES:	CC(=CCCC1(C)C2CC3C(C2)C31C)COC(=O)Nc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	384.47
CAS:	100264-27-5

Physical Properties

Property code	Value	Unit	Source
gf	379.88	kJ/mol	Joback Method
hf	-146.49	kJ/mol	Joback Method
hfus	52.68	kJ/mol	Joback Method
hvap	96.20	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	5.552		Crippen Method
mcvol	295.040	ml/mol	McGowan Method
pc	1572.21	kPa	Joback Method
tb	1019.58	K	Joback Method
tc	1265.17	K	Joback Method
tf	726.21	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1070.08	J/molxK	1019.58	Joback Method
cpg	1100.75	J/molxK	1060.51	Joback Method
cpg	1134.03	J/molxK	1101.44	Joback Method
cpg	1170.38	J/molxK	1142.37	Joback Method
cpg	1210.29	J/molxK	1183.30	Joback Method
cpg	1254.23	J/molxK	1224.24	Joback Method
cpg	1302.69	J/molxK	1265.17	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=C100264275&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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