

O-nitro carbanilic acid, cedrol ester

Inchi:	InChI=1S/C22H30N2O4/c1-14-9-10-17-20(2,3)18-13-22(14,17)12-11-21(18,4)28-19(25)2
InchiKey:	HFRKDCZGTM MNIX-UHFFFAOYSA-N
Formula:	C22H30N2O4
SMILES:	CC1CCC2C(C)(C)C3CC12CCC3(C)OC(=O)Nc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	386.48
CAS:	104913-49-7

Physical Properties

Property code	Value	Unit	Source
gf	246.61	kJ/mol	Joback Method
hf	-283.66	kJ/mol	Joback Method
hfus	40.16	kJ/mol	Joback Method
hvap	95.39	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	5.774		Crippen Method
mcvol	299.340	ml/mol	McGowan Method
pc	1643.09	kPa	Joback Method
tb	1028.19	K	Joback Method
tc	1288.62	K	Joback Method
tf	750.83	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1131.17	J/molxK	1028.19	Joback Method
cpg	1169.08	J/molxK	1071.60	Joback Method
cpg	1210.50	J/molxK	1115.00	Joback Method
cpg	1256.07	J/molxK	1158.41	Joback Method
cpg	1306.39	J/molxK	1201.81	Joback Method
cpg	1362.09	J/molxK	1245.22	Joback Method
cpg	1423.79	J/molxK	1288.62	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=C104913497&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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