

O-nitro carbanilic acid, cinnamyl ester

Inchi:	InChI=1S/C16H14N2O4/c19-16(17-14-10-4-5-11-15(14)18(20)21)22-12-6-9-13-7-2-1-3-8
InchiKey:	OZCYFXADSJBCHE-RMKNXTFCSA-N
Formula:	C16H14N2O4
SMILES:	O=C(Nc1ccccc1[N+](=O)[O-])OCC=Cc1ccccc1
Mol. weight [g/mol]:	298.29
CAS:	93014-31-4

Physical Properties

Property code	Value	Unit	Source
gf	270.27	kJ/mol	Joback Method
hf	3.15	kJ/mol	Joback Method
hfus	44.34	kJ/mol	Joback Method
hvap	88.56	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	3.857		Crippen Method
mcvol	219.320	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
tb	906.28	K	Joback Method
tc	1162.61	K	Joback Method
tf	598.79	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.41	J/molxK	906.28	Joback Method
cpg	652.70	J/molxK	949.00	Joback Method
cpg	662.89	J/molxK	991.72	Joback Method
cpg	672.10	J/molxK	1034.45	Joback Method
cpg	680.42	J/molxK	1077.17	Joback Method
cpg	687.95	J/molxK	1119.89	Joback Method
cpg	694.81	J/molxK	1162.61	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93014314&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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