O-nitro carbanilic acid, linalyl ester

Inchi: InChI=1S/C17H22N2O4/c1-5-17(4,12-8-9-13(2)3)23-16(20)18-14-10-6-7-11-15(14)19(21
InchiKey: CULRFNNDFRVPHV-UHFFFAOYSA-N
Formula: C17H22N2O4
SMILES: C=CC(C)(CCC=C(C)C)OC(=O)Nc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 318.37
CAS: 94709-92-9

Physical Properties

Property code	Value	Unit	Source
gf	248.41	kJ/mol	Joback Method
hf	-147.13	kJ/mol	Joback Method
hfus	42.88	kJ/mol	Joback Method
hvap	86.63	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	4.834		Crippen Method
mcvol	252.870	ml/mol	McGowan Method
pc	1818.50	kPa	Joback Method
tb	895.81	K	Joback Method
tc	1131.07	K	Joback Method
tf	570.34	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.84	J/mol×K	895.81	Joback Method
cpg	787.30	J/mol×K	935.02	Joback Method
cpg	799.80	J/mol×K	974.23	Joback Method
cpg	811.46	J/mol×K	1013.44	Joback Method
cpg	822.37	J/mol×K	1052.65	Joback Method
cpg	832.65	J/mol×K	1091.86	Joback Method
cpg	842.40	J/mol×K	1131.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94709929&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume