O-nitro carbanilic acid, phenethyl ester

Inchi: InChI=1S/C15H14N2O4/c18-15(21-11-10-12-6-2-1-3-7-12)16-13-8-4-5-9-14(13)17(19)20
InchiKey: PSODNDPTSGGTNE-UHFFFAOYSA-N
Formula: C15H14N2O4
SMILES: O=C(Nc1ccccc1[N+](=O)[O-])OCCc1ccccc1
Mol. weight [g/mol]: 286.28
CAS: 93733-82-5

Physical Properties

Property code	Value	Unit	Source
gf	181.63	kJ/mol	Joback Method
hf	-93.43	kJ/mol	Joback Method
hfus	41.55	kJ/mol	Joback Method
hvap	86.38	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.386		Crippen Method
mcvol	209.530	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
tb	879.24	K	Joback Method
tc	1131.87	K	Joback Method
tf	592.60	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.17	J/mol×K	879.24	Joback Method
cpg	625.59	J/mol×K	921.34	Joback Method
cpg	635.81	J/mol×K	963.45	Joback Method
cpg	644.87	J/mol×K	1005.55	Joback Method
cpg	652.87	J/mol×K	1047.66	Joback Method
cpg	659.86	J/mol×K	1089.76	Joback Method
cpg	665.93	J/mol×K	1131.87	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=C93733825&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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