O-nitro carbanilic acid, 4-terpinenol ester

Inchi: InChI=1S/C17H22N2O4/c1-11(2)13-9-8-12(3)10-16(13)23-17(20)18-14-6-4-5-7-15(14)19
InchiKey: TZNDTJVJZCHKMM-UHFFFAOYSA-N
Formula: C17H22N2O4
SMILES: CC1=CCC(C(C)C)C(OC(=O)Nc2ccccc2[N+](=O)[O-])C1
Mol. weight [g/mol]: 318.37

Physical Properties

Property code	Value	Unit	Source
gf	120.69	kJ/mol	Joback Method
hf	-296.23	kJ/mol	Joback Method
hfus	42.90	kJ/mol	Joback Method
hvap	89.24	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.524		Crippen Method
mcvol	246.310	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
tb	916.90	K	Joback Method
tc	1162.47	K	Joback Method
tf	590.14	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.65	J/mol×K	916.90	Joback Method
cpg	810.63	J/mol×K	957.83	Joback Method
cpg	823.03	J/mol×K	998.76	Joback Method
cpg	833.90	J/mol×K	1039.69	Joback Method
cpg	843.28	J/mol×K	1080.61	Joback Method
cpg	851.23	J/mol×K	1121.54	Joback Method
cpg	857.80	J/mol×K	1162.47	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6002504&Units=SI

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