Phenylthioacetic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C14H11NO4S/c16-14(10-20-13-4-2-1-3-5-13)19-12-8-6-11(7-9-12)15(17)18/h1
InchiKey: BMVZFCUYQCRMRJ-UHFFFAOYSA-N
Formula: C14H11NO4S
SMILES: O=C(CSc1ccccc1)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 289.31

Physical Properties

Property code	Value	Unit	Source
gf	116.94	kJ/mol	Joback Method
hf	-84.39	kJ/mol	Joback Method
hfus	37.99	kJ/mol	Joback Method
hvap	84.54	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.292		Crippen Method
mcvol	201.810	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	2412.00		NIST Webbook
tb	874.97	K	Joback Method
tc	1149.95	K	Joback Method
tf	563.07	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.09	J/mol×K	874.97	Joback Method
cpg	566.75	J/mol×K	920.80	Joback Method
cpg	575.98	J/mol×K	966.63	Joback Method
cpg	583.86	J/mol×K	1012.46	Joback Method
cpg	590.45	J/mol×K	1058.29	Joback Method
cpg	595.80	J/mol×K	1104.12	Joback Method
cpg	599.99	J/mol×K	1149.95	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=U307779&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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