Phenylthioacetic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C15H11NO2S/c16-10-12-6-8-13(9-7-12)18-15(17)11-19-14-4-2-1-3-5-14/h1-9H
InchiKey: DQJSGKNXEASBDL-UHFFFAOYSA-N
Formula: C15H11NO2S
SMILES: N#Cc1ccc(OC(=O)CSc2ccccc2)cc1
Mol. weight [g/mol]: 269.32

Physical Properties

Property code	Value	Unit	Source
gf	222.99	kJ/mol	Joback Method
hf	70.61	kJ/mol	Joback Method
hfus	30.72	kJ/mol	Joback Method
hvap	80.65	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.256		Crippen Method
mcvol	199.860	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	2275.00		NIST Webbook
tb	848.09	K	Joback Method
tc	1110.60	K	Joback Method
tf	495.72	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.66	J/mol×K	848.09	Joback Method
cpg	542.42	J/mol×K	891.84	Joback Method
cpg	551.91	J/mol×K	935.59	Joback Method
cpg	560.19	J/mol×K	979.35	Joback Method
cpg	567.30	J/mol×K	1023.10	Joback Method
cpg	573.29	J/mol×K	1066.85	Joback Method
cpg	578.20	J/mol×K	1110.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307777&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

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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