Phenylthioacetamide, N-(2-fluorophenyl)-

Inchi: InChI=1S/C14H12FNOS/c15-12-8-4-5-9-13(12)16-14(17)10-18-11-6-2-1-3-7-11/h1-9H,10
InchiKey: GGSNUOCLYCAAKJ-UHFFFAOYSA-N
Formula: C14H12FNOS
SMILES: O=C(CSc1ccccc1)Nc1ccccc1F
Mol. weight [g/mol]: 261.31

Physical Properties

Property code	Value	Unit	Source
gf	80.97	kJ/mol	Joback Method
hf	-84.05	kJ/mol	Joback Method
hfus	33.62	kJ/mol	Joback Method
hvap	71.15	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.556		Crippen Method
mcvol	190.270	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpol	2097.00		NIST Webbook
tb	750.15	K	Joback Method
tc	998.78	K	Joback Method
tf	450.48	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.78	J/mol×K	750.15	Joback Method
cpg	511.96	J/mol×K	791.59	Joback Method
cpg	523.92	J/mol×K	833.03	Joback Method
cpg	534.72	J/mol×K	874.47	Joback Method
cpg	544.43	J/mol×K	915.90	Joback Method
cpg	553.13	J/mol×K	957.34	Joback Method
cpg	560.87	J/mol×K	998.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308158&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