

Acetamide, N-(4-fluorophenyl)-2-phenylthio-

Inchi:	InChI=1S/C14H12FNOS/c15-11-6-8-12(9-7-11)16-14(17)10-18-13-4-2-1-3-5-13/h1-9H,10
InchiKey:	BZOQHGGJUFYYMFB-UHFFFAOYSA-N
Formula:	C14H12FNOS
SMILES:	O=C(CSc1cccc1)Nc1ccc(F)cc1
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
mvol	190.270	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rmpol	2157.00		NIST Webbook
rmpol	2157.00		NIST Webbook
tb	750.15	K	Joback Method
tc	998.78	K	Joback Method
tf	450.48	K	Joback Method
vc	0.717	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.78	J/molxK	750.15	Joback Method
cpg	511.96	J/molxK	791.59	Joback Method
cpg	523.92	J/molxK	833.03	Joback Method
cpg	534.72	J/molxK	874.47	Joback Method
cpg	544.43	J/molxK	915.90	Joback Method
cpg	553.13	J/molxK	957.34	Joback Method
cpg	560.87	J/molxK	998.78	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=U307205&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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