

Acetamide, N-(3-methylphenyl)-2-phenylthio-

Inchi:	InChI=1S/C15H15NOS/c1-12-6-5-7-13(10-12)16-15(17)11-18-14-8-3-2-4-9-14/h2-10H,11
InchiKey:	YQSBNGWFXIALFT-UHFFFAOYSA-N
Formula:	C15H15NOS
SMILES:	<chem>Cc1cccc(N=C(O)CSc2ccccc2)c1</chem>
Mol. weight [g/mol]:	257.35

Physical Properties

Property code	Value	Unit	Source
hf	70.73	kJ/mol	Joback Method
hvap	81.09	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	4.375		Crippen Method
mcvol	202.590	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	2270.00		NIST Webbook
tb	838.46	K	Joback Method
tc	1084.86	K	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=U307206&Units=SI

Legend

hf:	Enthalpy of formation 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

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