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

Inchi: InChI=1S/C15H15NO2S/c1-18-13-9-7-12(8-10-13)16-15(17)11-19-14-5-3-2-4-6-14/h2-10
InchiKey: QANIOCTWVUAMON-UHFFFAOYSA-N
Formula: C15H15NO2S
SMILES: COc1ccc(NC(=O)CSc2ccccc2)cc1
Mol. weight [g/mol]: 273.35

Physical Properties

Property code	Value	Unit	Source
gf	179.20	kJ/mol	Joback Method
hf	-40.80	kJ/mol	Joback Method
hfus	34.31	kJ/mol	Joback Method
hvap	76.61	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.426		Crippen Method
mcvol	208.460	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	2464.00		NIST Webbook
rinpol	2464.00		NIST Webbook
tb	796.18	K	Joback Method
tc	1046.47	K	Joback Method
tf	483.39	K	Joback Method
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.58	J/mol×K	796.18	Joback Method
cpg	583.24	J/mol×K	837.89	Joback Method
cpg	595.57	J/mol×K	879.61	Joback Method
cpg	606.61	J/mol×K	921.32	Joback Method
cpg	616.41	J/mol×K	963.04	Joback Method
cpg	625.02	J/mol×K	1004.75	Joback Method
cpg	632.50	J/mol×K	1046.47	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=U307208&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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