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

Inchi: InChI=1S/C14H12BrNOS/c15-11-6-8-12(9-7-11)16-14(17)10-18-13-4-2-1-3-5-13/h1-9H,1
InchiKey: YQSKUBFOMQDONL-UHFFFAOYSA-N
Formula: C14H12BrNOS
SMILES: O=C(CSc1ccccc1)Nc1ccc(Br)cc1
Mol. weight [g/mol]: 322.22

Physical Properties

Property code	Value	Unit	Source
gf	290.10	kJ/mol	Joback Method
hf	138.39	kJ/mol	Joback Method
hfus	35.82	kJ/mol	Joback Method
hvap	78.41	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.180		Crippen Method
mcvol	206.000	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
rinpol	2504.00		NIST Webbook
tb	817.04	K	Joback Method
tc	1086.22	K	Joback Method
tf	509.69	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.95	J/mol×K	817.04	Joback Method
cpg	533.81	J/mol×K	861.90	Joback Method
cpg	544.45	J/mol×K	906.77	Joback Method
cpg	553.96	J/mol×K	951.63	Joback Method
cpg	562.46	J/mol×K	996.49	Joback Method
cpg	570.03	J/mol×K	1041.35	Joback Method
cpg	576.80	J/mol×K	1086.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307209&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