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

Inchi: InChI=1S/C14H12BrNO/c15-12-6-8-13(9-7-12)16-14(17)10-11-4-2-1-3-5-11/h1-9H,10H2
InchiKey: XFXSNNWNLVLUOY-UHFFFAOYSA-N
Formula: C14H12BrNO
SMILES: O=C(Cc1ccccc1)Nc1ccc(Br)cc1
Mol. weight [g/mol]: 290.15

Physical Properties

Property code	Value	Unit	Source
gf	256.98	kJ/mol	Joback Method
hf	96.52	kJ/mol	Joback Method
hfus	31.69	kJ/mol	Joback Method
hvap	71.59	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.630		Crippen Method
mcvol	189.650	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
rinpol	2265.00		NIST Webbook
tb	748.26	K	Joback Method
tc	1003.03	K	Joback Method
tf	475.29	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.80	J/mol×K	748.26	Joback Method
cpg	487.72	J/mol×K	790.72	Joback Method
cpg	499.50	J/mol×K	833.18	Joback Method
cpg	510.21	J/mol×K	875.65	Joback Method
cpg	519.98	J/mol×K	918.11	Joback Method
cpg	528.89	J/mol×K	960.57	Joback Method
cpg	537.05	J/mol×K	1003.03	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=U307145&Units=SI

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