4'-BROMO-2'-PHENYLACETANILIDE

Other names: 2-acetamido-5-bromo-biphenyl
Inchi: InChI=1S/C14H12BrNO/c1-10(17)16-14-8-7-12(15)9-13(14)11-5-3-2-4-6-11/h2-9H,1H3,(
InchiKey: JUQGQHKZFREBLC-UHFFFAOYSA-N
Formula: C14H12BrNO
SMILES: CC(=O)Nc1ccc(Br)cc1-c1ccccc1
Mol. weight [g/mol]: 290.16

Physical Properties

Property code	Value	Unit	Source
hfus	31.30	kJ/mol	Joback Method
ie	8.01	eV	Cheméo Relay (1.0)
log10ws	-4.32		Cheméo Relay (1.0)
logp	4.075		Crippen Method
mcvol	189.650	ml/mol	McGowan Method
tb	643.91	K	Cheméo Relay (1.0)
tf	366.29	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.27	J/mol×K	753.24	Joback Method
cpg	486.07	J/mol×K	795.83	Joback Method
cpg	497.75	J/mol×K	838.42	Joback Method
cpg	508.40	J/mol×K	881.01	Joback Method
cpg	518.11	J/mol×K	923.60	Joback Method
cpg	526.97	J/mol×K	966.19	Joback Method
cpg	535.06	J/mol×K	1008.78	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7147526&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point