N,n-diphenyl-1-bromo-acetamide

Inchi: InChI=1S/C14H12BrNO/c15-11-14(17)16(12-7-3-1-4-8-12)13-9-5-2-6-10-13/h1-10H,11H
InchiKey: CIGSKJKGTWNQAX-UHFFFAOYSA-N
Formula: C14H12BrNO
SMILES: O=C(CBr)N(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 290.15
CAS: 6335-34-8

Physical Properties

Property code	Value	Unit	Source
gf	288.00	kJ/mol	Joback Method
hf	122.05	kJ/mol	Joback Method
hfus	30.00	kJ/mol	Joback Method
hvap	66.53	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.746		Crippen Method
mcvol	189.650	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
tb	705.55	K	Joback Method
tc	959.02	K	Joback Method
tf	442.58	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.36	J/mol×K	705.55	Joback Method
cpg	479.42	J/mol×K	747.80	Joback Method
cpg	492.19	J/mol×K	790.04	Joback Method
cpg	503.79	J/mol×K	832.29	Joback Method
cpg	514.34	J/mol×K	874.53	Joback Method
cpg	523.96	J/mol×K	916.78	Joback Method
cpg	532.78	J/mol×K	959.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6335348&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume