Pentanamide, N-(4-bromophenyl)-

Inchi: InChI=1S/C11H14BrNO/c1-2-3-4-11(14)13-10-7-5-9(12)6-8-10/h5-8H,2-4H2,1H3,(H,13,1
InchiKey: BVSHEOSLHJDADE-UHFFFAOYSA-N
Formula: C11H14BrNO
SMILES: CCCCC(=O)Nc1ccc(Br)cc1
Mol. weight [g/mol]: 256.14

Physical Properties

Property code	Value	Unit	Source
gf	119.31	kJ/mol	Joback Method
hf	-78.09	kJ/mol	Joback Method
hfus	29.88	kJ/mol	Joback Method
hvap	62.64	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.578		Crippen Method
mcvol	171.140	ml/mol	McGowan Method
pc	3042.32	kPa	Joback Method
rinpol	1928.00		NIST Webbook
rinpol	1928.00		NIST Webbook
tb	652.94	K	Joback Method
tc	877.40	K	Joback Method
tf	415.06	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.00	J/mol×K	652.94	Joback Method
cpg	422.02	J/mol×K	690.35	Joback Method
cpg	434.15	J/mol×K	727.76	Joback Method
cpg	445.44	J/mol×K	765.17	Joback Method
cpg	455.94	J/mol×K	802.58	Joback Method
cpg	465.70	J/mol×K	839.99	Joback Method
cpg	474.77	J/mol×K	877.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306894&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