Octanamide, N-(4-bromophenyl)-

Inchi: InChI=1S/C14H20BrNO/c1-2-3-4-5-6-7-14(17)16-13-10-8-12(15)9-11-13/h8-11H,2-7H2,1
InchiKey: KBXUYPJOGOGXDD-UHFFFAOYSA-N
Formula: C14H20BrNO
SMILES: CCCCCCCC(=O)Nc1ccc(Br)cc1
Mol. weight [g/mol]: 298.22

Physical Properties

Property code	Value	Unit	Source
gf	144.57	kJ/mol	Joback Method
hf	-140.01	kJ/mol	Joback Method
hfus	37.65	kJ/mol	Joback Method
hvap	69.31	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.748		Crippen Method
mcvol	213.410	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
rinpol	2253.00		NIST Webbook
tb	721.58	K	Joback Method
tc	935.27	K	Joback Method
tf	448.87	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.56	J/mol×K	721.58	Joback Method
cpg	578.10	J/mol×K	757.19	Joback Method
cpg	591.71	J/mol×K	792.81	Joback Method
cpg	604.43	J/mol×K	828.42	Joback Method
cpg	616.32	J/mol×K	864.04	Joback Method
cpg	627.44	J/mol×K	899.65	Joback Method
cpg	637.82	J/mol×K	935.27	Joback Method

Sources

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=U306927&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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