Hexanamide, N-(4-bromophenyl)-

Inchi: InChI=1S/C12H16BrNO/c1-2-3-4-5-12(15)14-11-8-6-10(13)7-9-11/h6-9H,2-5H2,1H3,(H,1
InchiKey: YWADRQJXUXOXIV-UHFFFAOYSA-N
Formula: C12H16BrNO
SMILES: CCCCCC(=O)Nc1ccc(Br)cc1
Mol. weight [g/mol]: 270.17

Physical Properties

Property code	Value	Unit	Source
gf	127.73	kJ/mol	Joback Method
hf	-98.73	kJ/mol	Joback Method
hfus	32.47	kJ/mol	Joback Method
hvap	64.86	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.968		Crippen Method
mcvol	185.230	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	2036.00		NIST Webbook
tb	675.82	K	Joback Method
tc	896.31	K	Joback Method
tf	426.33	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.19	J/mol×K	675.82	Joback Method
cpg	472.79	J/mol×K	712.57	Joback Method
cpg	485.49	J/mol×K	749.32	Joback Method
cpg	497.33	J/mol×K	786.06	Joback Method
cpg	508.37	J/mol×K	822.81	Joback Method
cpg	518.64	J/mol×K	859.56	Joback Method
cpg	528.21	J/mol×K	896.31	Joback Method

Sources

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=U307290&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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