Cyclopentanecarboxamide, N-(4-bromophenyl)-

Inchi: InChI=1S/C12H14BrNO/c13-10-5-7-11(8-6-10)14-12(15)9-3-1-2-4-9/h5-9H,1-4H2,(H,14,1

InchiKey: XPDHLCLPWLLADG-UHFFFAOYSA-N

Formula: C12H14BrNO

SMILES: O=C(Nc1ccc(Br)cc1)C1CCCC1

Mol. weight [g/mol]: 268.15

Physical Properties

Property code	Value	Unit	Source
gf	164.28	kJ/mol	Joback Method
hf	-38.25	kJ/mol	Joback Method
hfus	26.41	kJ/mol	Joback Method
hvap	65.12	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.578		Crippen Method
mcvol	174.370	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
rinpol	2093.00		NIST Webbook
tb	691.10	K	Joback Method
tc	941.80	K	Joback Method
tf	437.23	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.67	J/mol×K	691.10	Joback Method
cpg	463.06	J/mol×K	732.88	Joback Method
cpg	477.18	J/mol×K	774.67	Joback Method
cpg	490.11	J/mol×K	816.45	Joback Method
cpg	501.94	J/mol×K	858.24	Joback Method
cpg	512.77	J/mol×K	900.02	Joback Method
cpg	522.68	J/mol×K	941.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307028&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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