Cyclobutanecarboxamide, N-(4-bromophenyl)-

Inchi: InChI=1S/C11H12BrNO/c12-9-4-6-10(7-5-9)13-11(14)8-2-1-3-8/h4-8H,1-3H2,(H,13,14)
InchiKey: BGSGLQBVMIAUKC-UHFFFAOYSA-N
Formula: C11H12BrNO
SMILES: O=C(Nc1ccc(Br)cc1)C1CCC1
Mol. weight [g/mol]: 254.12

Physical Properties

Property code	Value	Unit	Source
gf	167.96	kJ/mol	Joback Method
hf	-11.45	kJ/mol	Joback Method
hfus	25.92	kJ/mol	Joback Method
hvap	62.72	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.188		Crippen Method
mcvol	160.280	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
rinpol	1984.00		NIST Webbook
tb	663.95	K	Joback Method
tc	912.09	K	Joback Method
tf	429.48	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.06	J/mol×K	663.95	Joback Method
cpg	409.14	J/mol×K	705.31	Joback Method
cpg	422.07	J/mol×K	746.66	Joback Method
cpg	433.95	J/mol×K	788.02	Joback Method
cpg	444.86	J/mol×K	829.38	Joback Method
cpg	454.90	J/mol×K	870.73	Joback Method
cpg	464.17	J/mol×K	912.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307050&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