Cyclohexanecarboxamide, N-(4-bromophenyl)-

Inchi: InChI=1S/C13H16BrNO/c14-11-6-8-12(9-7-11)15-13(16)10-4-2-1-3-5-10/h6-10H,1-5H2,(
InchiKey: JENRJNSQQXLAFZ-UHFFFAOYSA-N
Formula: C13H16BrNO
SMILES: O=C(Nc1ccc(Br)cc1)C1CCCCC1
Mol. weight [g/mol]: 282.18

Physical Properties

Property code	Value	Unit	Source
gf	160.60	kJ/mol	Joback Method
hf	-65.05	kJ/mol	Joback Method
hfus	26.90	kJ/mol	Joback Method
hvap	67.52	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.968		Crippen Method
mcvol	188.460	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
rinpol	2191.00		NIST Webbook
tb	718.25	K	Joback Method
tc	971.31	K	Joback Method
tf	444.98	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.33	J/mol×K	718.25	Joback Method
cpg	518.88	J/mol×K	760.43	Joback Method
cpg	534.00	J/mol×K	802.60	Joback Method
cpg	547.80	J/mol×K	844.78	Joback Method
cpg	560.35	J/mol×K	886.96	Joback Method
cpg	571.74	J/mol×K	929.13	Joback Method
cpg	582.05	J/mol×K	971.31	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306949&Units=SI

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