Cyclopropanecarboxamide, N-(4-bromophenyl)-

Inchi: InChI=1S/C10H10BrNO/c11-8-3-5-9(6-4-8)12-10(13)7-1-2-7/h3-7H,1-2H2,(H,12,13)
InchiKey: CYBVEZPTHHVBTO-UHFFFAOYSA-N
Formula: C10H10BrNO
SMILES: O=C(Nc1ccc(Br)cc1)C1CC1
Mol. weight [g/mol]: 240.10

Physical Properties

Property code	Value	Unit	Source
gf	171.64	kJ/mol	Joback Method
hf	15.35	kJ/mol	Joback Method
hfus	25.43	kJ/mol	Joback Method
hvap	60.32	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.798		Crippen Method
mcvol	146.190	ml/mol	McGowan Method
pc	3970.51	kPa	Joback Method
rinpol	1888.00		NIST Webbook
tb	636.80	K	Joback Method
tc	882.14	K	Joback Method
tf	421.73	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.68	J/mol×K	636.80	Joback Method
cpg	357.30	J/mol×K	677.69	Joback Method
cpg	368.89	J/mol×K	718.58	Joback Method
cpg	379.53	J/mol×K	759.47	Joback Method
cpg	389.33	J/mol×K	800.36	Joback Method
cpg	398.39	J/mol×K	841.25	Joback Method
cpg	406.81	J/mol×K	882.14	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=U307189&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