Bromoacetic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C9H6BrNO2/c10-5-9(12)13-8-3-1-7(6-11)2-4-8/h1-4H,5H2
InchiKey: XKCMGGJNGDRKOD-UHFFFAOYSA-N
Formula: C9H6BrNO2
SMILES: N#Cc1ccc(OC(=O)CBr)cc1
Mol. weight [g/mol]: 240.05

Physical Properties

Property code	Value	Unit	Source
gf	41.26	kJ/mol	Joback Method
hf	-57.62	kJ/mol	Joback Method
hfus	22.30	kJ/mol	Joback Method
hvap	64.64	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	1.859		Crippen Method
mcvol	140.230	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
rinpol	1631.00		NIST Webbook
tb	681.51	K	Joback Method
tc	926.13	K	Joback Method
tf	427.08	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.47	J/mol×K	681.51	Joback Method
cpg	313.17	J/mol×K	722.28	Joback Method
cpg	321.17	J/mol×K	763.05	Joback Method
cpg	328.50	J/mol×K	803.82	Joback Method
cpg	335.19	J/mol×K	844.59	Joback Method
cpg	341.24	J/mol×K	885.36	Joback Method
cpg	346.70	J/mol×K	926.13	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=U308049&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