4-Cyanobenzoic acid, 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C14H7BrFNO2/c15-12-7-11(16)5-6-13(12)19-14(18)10-3-1-9(8-17)2-4-10/h1-7

InchiKey: NDDGFRXURFDMFK-UHFFFAOYSA-N

Formula: C14H7BrFNO2

SMILES: N#Cc1ccc(C(=O)Oc2ccc(F)cc2Br)cc1

Mol. weight [g/mol]: 320.11

Physical Properties

Property code	Value	Unit	Source
gf	-18.30	kJ/mol	Joback Method
hf	-143.34	kJ/mol	Joback Method
hfus	31.59	kJ/mol	Joback Method
hvap	78.55	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	3.679		Crippen Method
mcvol	188.690	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
rinpol	1987.70		NIST Webbook
tb	831.82	K	Joback Method
tc	1085.54	K	Joback Method
tf	535.48	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.83	J/mol×K	831.82	Joback Method
cpg	473.90	J/mol×K	874.11	Joback Method
cpg	482.04	J/mol×K	916.39	Joback Method
cpg	489.29	J/mol×K	958.68	Joback Method
cpg	495.71	J/mol×K	1000.97	Joback Method
cpg	501.33	J/mol×K	1043.26	Joback Method
cpg	506.20	J/mol×K	1085.54	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=U292659&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