3-Bromobenzoic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C14H8BrNO2/c15-12-3-1-2-11(8-12)14(17)18-13-6-4-10(9-16)5-7-13/h1-8H
InchiKey: ZMVITGJZOFYUBU-UHFFFAOYSA-N
Formula: C14H8BrNO2
SMILES: N#Cc1ccc(OC(=O)c2cccc(Br)c2)cc1
Mol. weight [g/mol]: 302.12

Physical Properties

Property code	Value	Unit	Source
gf	186.14	kJ/mol	Joback Method
hf	64.24	kJ/mol	Joback Method
hfus	28.90	kJ/mol	Joback Method
hvap	78.70	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	3.540		Crippen Method
mcvol	186.920	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	2230.00		NIST Webbook
tb	827.57	K	Joback Method
tc	1091.43	K	Joback Method
tf	522.37	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.21	J/mol×K	827.57	Joback Method
cpg	468.87	J/mol×K	871.55	Joback Method
cpg	477.53	J/mol×K	915.52	Joback Method
cpg	485.23	J/mol×K	959.50	Joback Method
cpg	492.05	J/mol×K	1003.48	Joback Method
cpg	498.04	J/mol×K	1047.46	Joback Method
cpg	503.26	J/mol×K	1091.43	Joback Method

Sources

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=U307552&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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