3-Bromobenzoic acid, pentafluorophenyl ester

Inchi: InChI=1S/C13H4BrF5O2/c14-6-3-1-2-5(4-6)13(20)21-12-10(18)8(16)7(15)9(17)11(12)19/
InchiKey: SUFAXCUTMNDIJO-UHFFFAOYSA-N
Formula: C13H4BrF5O2
SMILES: O=C(Oc1c(F)c(F)c(F)c(F)c1F)c1cccc(Br)c1
Mol. weight [g/mol]: 367.07

Physical Properties

Property code	Value	Unit	Source
gf	-968.03	kJ/mol	Joback Method
hf	-1106.43	kJ/mol	Joback Method
hfus	38.65	kJ/mol	Joback Method
hvap	64.56	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	4.364		Crippen Method
mcvol	180.300	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
rinpol	1786.00		NIST Webbook
rinpol	1786.00		NIST Webbook
tb	718.88	K	Joback Method
tc	931.20	K	Joback Method
tf	499.14	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.66	J/mol×K	718.88	Joback Method
cpg	440.84	J/mol×K	754.27	Joback Method
cpg	449.35	J/mol×K	789.65	Joback Method
cpg	457.20	J/mol×K	825.04	Joback Method
cpg	464.40	J/mol×K	860.43	Joback Method
cpg	470.96	J/mol×K	895.82	Joback Method
cpg	476.89	J/mol×K	931.20	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=U355182&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