3-Bromobenzoic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C12H7BrF8O2/c13-7-3-1-2-6(4-7)8(22)23-5-10(16,17)12(20,21)11(18,19)9(14)
InchiKey: PCXNEAYFCQQGHJ-UHFFFAOYSA-N
Formula: C12H7BrF8O2
SMILES: O=C(OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1cccc(Br)c1
Mol. weight [g/mol]: 415.07

Physical Properties

Property code	Value	Unit	Source
gf	-1619.06	kJ/mol	Joback Method
hf	-1884.83	kJ/mol	Joback Method
hfus	27.43	kJ/mol	Joback Method
hvap	50.02	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	4.777		Crippen Method
mcvol	195.280	ml/mol	McGowan Method
pc	2003.70	kPa	Joback Method
rinpol	1571.00		NIST Webbook
rinpol	1571.00		NIST Webbook
tb	632.10	K	Joback Method
tc	817.50	K	Joback Method
tf	392.88	K	Joback Method
vc	0.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.23	J/mol×K	632.10	Joback Method
cpg	520.10	J/mol×K	663.00	Joback Method
cpg	530.09	J/mol×K	693.90	Joback Method
cpg	539.26	J/mol×K	724.80	Joback Method
cpg	547.67	J/mol×K	755.70	Joback Method
cpg	555.38	J/mol×K	786.60	Joback Method
cpg	562.47	J/mol×K	817.50	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=U355179&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