2-Bromo-5-fluorobenzyl alcohol, chlorodifluoroacetate

Inchi: InChI=1S/C9H5BrClF3O2/c10-7-2-1-6(12)3-5(7)4-16-8(15)9(11,13)14/h1-3H,4H2
InchiKey: MPJCPBPMLDNWMA-UHFFFAOYSA-N
Formula: C9H5BrClF3O2
SMILES: O=C(OCc1cc(F)ccc1Br)C(F)(F)Cl
Mol. weight [g/mol]: 317.49

Physical Properties

Property code	Value	Unit	Source
gf	-695.07	kJ/mol	Joback Method
hf	-846.79	kJ/mol	Joback Method
hfus	26.42	kJ/mol	Joback Method
hvap	55.46	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.463		Crippen Method
mcvol	156.400	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	1404.00		NIST Webbook
rinpol	1404.00		NIST Webbook
tb	616.42	K	Joback Method
tc	833.23	K	Joback Method
tf	408.72	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.64	J/mol×K	616.42	Joback Method
cpg	349.73	J/mol×K	652.55	Joback Method
cpg	358.11	J/mol×K	688.69	Joback Method
cpg	365.81	J/mol×K	724.82	Joback Method
cpg	372.89	J/mol×K	760.96	Joback Method
cpg	379.37	J/mol×K	797.09	Joback Method
cpg	385.29	J/mol×K	833.23	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=U376075&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