Benzyl alcohol, chlorodifluoroacetate

Inchi: InChI=1S/C9H7ClF2O2/c10-9(11,12)8(13)14-6-7-4-2-1-3-5-7/h1-5H,6H2
InchiKey: FMBDRDJDLSYKAV-UHFFFAOYSA-N
Formula: C9H7ClF2O2
SMILES: O=C(OCc1ccccc1)C(F)(F)Cl
Mol. weight [g/mol]: 220.60

Physical Properties

Property code	Value	Unit	Source
gf	-495.32	kJ/mol	Joback Method
hf	-654.07	kJ/mol	Joback Method
hfus	18.84	kJ/mol	Joback Method
hvap	48.52	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.561		Crippen Method
mcvol	137.130	ml/mol	McGowan Method
pc	3042.32	kPa	Joback Method
rinpol	1177.00		NIST Webbook
rinpol	1177.00		NIST Webbook
tb	541.03	K	Joback Method
tc	753.37	K	Joback Method
tf	323.29	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.70	J/mol×K	541.03	Joback Method
cpg	313.14	J/mol×K	576.42	Joback Method
cpg	323.75	J/mol×K	611.81	Joback Method
cpg	333.56	J/mol×K	647.20	Joback Method
cpg	342.61	J/mol×K	682.59	Joback Method
cpg	350.95	J/mol×K	717.98	Joback Method
cpg	358.61	J/mol×K	753.37	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=U376217&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