2,3,4,5-Tetrafluorobenzyl alcohol, chlorodifluoroacetate

Inchi: InChI=1S/C9H3ClF6O2/c10-9(15,16)8(17)18-2-3-1-4(11)6(13)7(14)5(3)12/h1H,2H2
InchiKey: ZMVNXEPMQCKYLS-UHFFFAOYSA-N
Formula: C9H3ClF6O2
SMILES: O=C(OCc1cc(F)c(F)c(F)c1F)C(F)(F)Cl
Mol. weight [g/mol]: 292.56

Physical Properties

Property code	Value	Unit	Source
gf	-1313.08	kJ/mol	Joback Method
hf	-1484.39	kJ/mol	Joback Method
hfus	29.60	kJ/mol	Joback Method
hvap	47.89	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.118		Crippen Method
mcvol	144.210	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
rinpol	1125.00		NIST Webbook
rinpol	1125.00		NIST Webbook
tb	558.03	K	Joback Method
tc	737.52	K	Joback Method
tf	375.73	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.06	J/mol×K	558.03	Joback Method
cpg	340.40	J/mol×K	587.94	Joback Method
cpg	348.27	J/mol×K	617.86	Joback Method
cpg	355.69	J/mol×K	647.77	Joback Method
cpg	362.66	J/mol×K	677.69	Joback Method
cpg	369.19	J/mol×K	707.60	Joback Method
cpg	375.31	J/mol×K	737.52	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=U376274&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