3,4,5-Trifluorobenzyl alcohol, chloro(difluoro)acetate

Inchi: InChI=1S/C9H4ClF5O2/c10-9(14,15)8(16)17-3-4-1-5(11)7(13)6(12)2-4/h1-2H,3H2
InchiKey: ABWXEBWMURTTSX-UHFFFAOYSA-N
Formula: C9H4ClF5O2
SMILES: O=C(OCc1cc(F)c(F)c(F)c1)C(F)(F)Cl
Mol. weight [g/mol]: 274.57

Physical Properties

Property code	Value	Unit	Source
gf	-1108.64	kJ/mol	Joback Method
hf	-1276.81	kJ/mol	Joback Method
hfus	26.91	kJ/mol	Joback Method
hvap	48.05	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	2.979		Crippen Method
mcvol	142.440	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
rinpol	1171.00		NIST Webbook
rinpol	1171.00		NIST Webbook
tb	553.78	K	Joback Method
tc	740.45	K	Joback Method
tf	362.62	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.60	J/mol×K	553.78	Joback Method
cpg	333.61	J/mol×K	584.89	Joback Method
cpg	342.08	J/mol×K	616.00	Joback Method
cpg	350.03	J/mol×K	647.11	Joback Method
cpg	357.47	J/mol×K	678.22	Joback Method
cpg	364.41	J/mol×K	709.34	Joback Method
cpg	370.88	J/mol×K	740.45	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=U376071&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