3,5-Dichlorobenzyl alcohol, chlorodifluoroacetate

Inchi: InChI=1S/C9H5Cl3F2O2/c10-6-1-5(2-7(11)3-6)4-16-8(15)9(12,13)14/h1-3H,4H2
InchiKey: VFKTXFRHYLUUNF-UHFFFAOYSA-N
Formula: C9H5Cl3F2O2
SMILES: O=C(OCc1cc(Cl)cc(Cl)c1)C(F)(F)Cl
Mol. weight [g/mol]: 289.49

Physical Properties

Property code	Value	Unit	Source
gf	-538.44	kJ/mol	Joback Method
hf	-708.49	kJ/mol	Joback Method
hfus	26.45	kJ/mol	Joback Method
hvap	58.61	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.868		Crippen Method
mcvol	161.610	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
rinpol	1503.00		NIST Webbook
rinpol	1503.00		NIST Webbook
tb	625.85	K	Joback Method
tc	848.15	K	Joback Method
tf	408.17	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.89	J/mol×K	625.85	Joback Method
cpg	353.90	J/mol×K	662.90	Joback Method
cpg	362.19	J/mol×K	699.95	Joback Method
cpg	369.78	J/mol×K	737.00	Joback Method
cpg	376.72	J/mol×K	774.05	Joback Method
cpg	383.04	J/mol×K	811.10	Joback Method
cpg	388.78	J/mol×K	848.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376102&Units=SI
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

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