3-Chloro-2-nitrobenzyl alcohol, chlorodifluoroacetate

Inchi: InChI=1S/C9H5Cl2F2NO4/c10-6-3-1-2-5(7(6)14(16)17)4-18-8(15)9(11,12)13/h1-3H,4H2

InchiKey: JISKAOPKQLJDMM-UHFFFAOYSA-N

Formula: C9H5Cl2F2NO4

SMILES: O=C(OCc1cccc(Cl)c1[N+](=O)[O-])C(F)(F)Cl

Mol. weight [g/mol]: 300.04

Physical Properties

Property code	Value	Unit	Source
gf	-490.96	kJ/mol	Joback Method
hf	-703.51	kJ/mol	Joback Method
hfus	33.62	kJ/mol	Joback Method
hvap	70.81	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.123		Crippen Method
mcvol	166.790	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
rinpol	1651.00		NIST Webbook
rinpol	1651.00		NIST Webbook
tb	740.26	K	Joback Method
tc	979.89	K	Joback Method
tf	521.86	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.13	J/mol×K	740.26	Joback Method
cpg	412.45	J/mol×K	780.20	Joback Method
cpg	419.95	J/mol×K	820.14	Joback Method
cpg	426.69	J/mol×K	860.08	Joback Method
cpg	432.70	J/mol×K	900.01	Joback Method
cpg	438.05	J/mol×K	939.95	Joback Method
cpg	442.78	J/mol×K	979.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376112&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