2-Fluoro-5-nitrobenzyl alcohol, chlorodifluoroacetate

Inchi: InChI=1S/C9H5ClF3NO4/c10-9(12,13)8(15)18-4-5-3-6(14(16)17)1-2-7(5)11/h1-3H,4H2

InchiKey: DKPARYQUTXKKFW-UHFFFAOYSA-N

Formula: C9H5ClF3NO4

SMILES: O=C(OCc1cc([N+](=O)[O-])ccc1F)C(F)(F)Cl

Mol. weight [g/mol]: 283.59

Physical Properties

Property code	Value	Unit	Source
gf	-673.84	kJ/mol	Joback Method
hf	-883.88	kJ/mol	Joback Method
hfus	32.50	kJ/mol	Joback Method
hvap	65.61	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	2.609		Crippen Method
mcvol	156.320	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
rinpol	1563.00		NIST Webbook
rinpol	1563.00		NIST Webbook
tb	702.10	K	Joback Method
tc	929.01	K	Joback Method
tf	492.53	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.88	J/mol×K	702.10	Joback Method
cpg	401.77	J/mol×K	739.92	Joback Method
cpg	409.87	J/mol×K	777.74	Joback Method
cpg	417.23	J/mol×K	815.56	Joback Method
cpg	423.88	J/mol×K	853.38	Joback Method
cpg	429.86	J/mol×K	891.19	Joback Method
cpg	435.22	J/mol×K	929.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376135&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