

5-Chloro-2-nitrobenzyl alcohol, chlorodifluoroacetate

Inchi:	InChI=1S/C9H5Cl2F2NO4/c10-6-1-2-7(14(16)17)5(3-6)4-18-8(15)9(11,12)13/h1-3H,4H2
InchiKey:	LESCSKZMPASYHW-UHFFFAOYSA-N
Formula:	C9H5Cl2F2NO4
SMILES:	O=C(OCc1cc(Cl)ccc1[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	1672.00		NIST Webbook
rinpol	1672.00		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/molxK	740.26	Joback Method
cpg	412.45	J/molxK	780.20	Joback Method
cpg	419.95	J/molxK	820.14	Joback Method
cpg	426.69	J/molxK	860.08	Joback Method
cpg	432.70	J/molxK	900.01	Joback Method
cpg	438.05	J/molxK	939.95	Joback Method
cpg	442.78	J/molxK	979.89	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U376124&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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