3,4-Difluorobenzyl alcohol, chlorodifluoroacetate

Inchi: InChI=1S/C9H5ClF4O2/c10-9(13,14)8(15)16-4-5-1-2-6(11)7(12)3-5/h1-3H,4H2

InchiKey: NSHFCEVUGAOUBP-UHFFFAOYSA-N

Formula: C9H5ClF4O2

SMILES: O=C(OCc1ccc(F)c(F)c1)C(F)(F)Cl

Mol. weight [g/mol]: 256.58

Physical Properties

Property code	Value	Unit	Source
gf	-904.20	kJ/mol	Joback Method
hf	-1069.23	kJ/mol	Joback Method
hfus	24.22	kJ/mol	Joback Method
hvap	48.20	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	2.840		Crippen Method
mcvol	140.670	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
rinpol	1191.00		NIST Webbook
rinpol	1191.00		NIST Webbook
tb	549.53	K	Joback Method
tc	744.04	K	Joback Method
tf	349.51	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.06	J/mol×K	549.53	Joback Method
cpg	326.81	J/mol×K	581.95	Joback Method
cpg	335.93	J/mol×K	614.37	Joback Method
cpg	344.45	J/mol×K	646.79	Joback Method
cpg	352.39	J/mol×K	679.20	Joback Method
cpg	359.77	J/mol×K	711.62	Joback Method
cpg	366.62	J/mol×K	744.04	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376132&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
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