4-(2-Hydroxyethyl)-2,2-dimethyl-1,3-dioxolane, chlorodifluoroacetate

Inchi: InChI=1S/C9H13ClF2O4/c1-8(2)15-5-6(16-8)3-4-14-7(13)9(10,11)12/h6H,3-5H2,1-2H3

InchiKey: KCPIJFSNJRKXHR-UHFFFAOYSA-N

Formula: C9H13ClF2O4

SMILES: CC1(C)OCC(CCOC(=O)C(F)(F)Cl)O1

Mol. weight [g/mol]: 258.65

Physical Properties

Property code	Value	Unit	Source
gf	-756.62	kJ/mol	Joback Method
hf	-1099.22	kJ/mol	Joback Method
hfus	29.46	kJ/mol	Joback Method
hvap	54.06	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.903		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
rinpol	1214.00		NIST Webbook
rinpol	1214.00		NIST Webbook
tb	579.10	K	Joback Method
tc	782.08	K	Joback Method
tf	380.57	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.95	J/mol×K	579.10	Joback Method
cpg	432.55	J/mol×K	612.93	Joback Method
cpg	445.30	J/mol×K	646.76	Joback Method
cpg	457.29	J/mol×K	680.59	Joback Method
cpg	468.62	J/mol×K	714.42	Joback Method
cpg	479.39	J/mol×K	748.25	Joback Method
cpg	489.69	J/mol×K	782.08	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=U376262&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

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