2,2-Dichloroethanol, chlorodifluoroacetate

Inchi: InChI=1S/C4H3Cl3F2O2/c5-2(6)1-11-3(10)4(7,8)9/h2H,1H2
InchiKey: OQBPYXLKTSMTLW-UHFFFAOYSA-N
Formula: C4H3Cl3F2O2
SMILES: O=C(OCC(Cl)Cl)C(F)(F)Cl
Mol. weight [g/mol]: 227.42

Physical Properties

Property code	Value	Unit	Source
gf	-676.13	kJ/mol	Joback Method
hf	-824.16	kJ/mol	Joback Method
hfus	16.72	kJ/mol	Joback Method
hvap	43.49	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.165		Crippen Method
mcvol	114.920	ml/mol	McGowan Method
pc	3341.24	kPa	Joback Method
rinpol	947.00		NIST Webbook
tb	474.37	K	Joback Method
tc	671.36	K	Joback Method
tf	285.36	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.77	J/mol×K	474.37	Joback Method
cpg	219.36	J/mol×K	507.20	Joback Method
cpg	225.50	J/mol×K	540.03	Joback Method
cpg	231.21	J/mol×K	572.86	Joback Method
cpg	236.51	J/mol×K	605.70	Joback Method
cpg	241.41	J/mol×K	638.53	Joback Method
cpg	245.93	J/mol×K	671.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376211&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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