Cyclohexanemethanol, chlorodifluoroacetate

Inchi: InChI=1S/C9H13ClF2O2/c10-9(11,12)8(13)14-6-7-4-2-1-3-5-7/h7H,1-6H2
InchiKey: OKWLAXYAGXOAFE-UHFFFAOYSA-N
Formula: C9H13ClF2O2
SMILES: O=C(OCC1CCCCC1)C(F)(F)Cl
Mol. weight [g/mol]: 226.65

Physical Properties

Property code	Value	Unit	Source
gf	-583.28	kJ/mol	Joback Method
hf	-836.28	kJ/mol	Joback Method
hfus	16.63	kJ/mol	Joback Method
hvap	46.67	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.942		Crippen Method
mcvol	150.030	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
rinpol	1170.00		NIST Webbook
rinpol	1170.00		NIST Webbook
tb	533.90	K	Joback Method
tc	739.03	K	Joback Method
tf	304.25	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.29	J/mol×K	533.90	Joback Method
cpg	374.03	J/mol×K	568.09	Joback Method
cpg	388.79	J/mol×K	602.28	Joback Method
cpg	402.62	J/mol×K	636.46	Joback Method
cpg	415.54	J/mol×K	670.65	Joback Method
cpg	427.60	J/mol×K	704.84	Joback Method
cpg	438.81	J/mol×K	739.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376259&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

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