1-Cyclopentylethanol, chlorodifluoroacetate

Inchi: InChI=1S/C9H13ClF2O2/c1-6(7-4-2-3-5-7)14-8(13)9(10,11)12/h6-7H,2-5H2,1H3
InchiKey: VUZXFKJPYZZSQW-UHFFFAOYSA-N
Formula: C9H13ClF2O2
SMILES: CC(OC(=O)C(F)(F)Cl)C1CCCC1
Mol. weight [g/mol]: 226.65

Physical Properties

Property code	Value	Unit	Source
gf	-573.62	kJ/mol	Joback Method
hf	-835.40	kJ/mol	Joback Method
hfus	15.21	kJ/mol	Joback Method
hvap	46.11	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.940		Crippen Method
mcvol	150.030	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	1110.00		NIST Webbook
rinpol	1110.00		NIST Webbook
tb	529.19	K	Joback Method
tc	731.52	K	Joback Method
tf	292.77	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.17	J/mol×K	529.19	Joback Method
cpg	373.41	J/mol×K	562.91	Joback Method
cpg	387.71	J/mol×K	596.63	Joback Method
cpg	401.09	J/mol×K	630.35	Joback Method
cpg	413.61	J/mol×K	664.07	Joback Method
cpg	425.29	J/mol×K	697.80	Joback Method
cpg	436.17	J/mol×K	731.52	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=U376252&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