trans-2-Methylcyclohexanol, chlorodifluoroacetate

Inchi: InChI=1S/C9H13ClF2O2/c1-6-4-2-3-5-7(6)14-8(13)9(10,11)12/h6-7H,2-5H2,1H3
InchiKey: LBNMIKAZVLVNGN-UHFFFAOYSA-N
Formula: C9H13ClF2O2
SMILES: CC1CCCCC1OC(=O)C(F)(F)Cl
Mol. weight [g/mol]: 226.65

Physical Properties

Property code	Value	Unit	Source
gf	-590.99	kJ/mol	Joback Method
hf	-856.62	kJ/mol	Joback Method
hfus	17.70	kJ/mol	Joback Method
hvap	46.36	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.940		Crippen Method
mcvol	150.030	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	1112.00		NIST Webbook
rinpol	1112.00		NIST Webbook
tb	529.23	K	Joback Method
tc	734.20	K	Joback Method
tf	300.01	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.33	J/mol×K	529.23	Joback Method
cpg	375.48	J/mol×K	563.39	Joback Method
cpg	390.69	J/mol×K	597.55	Joback Method
cpg	404.96	J/mol×K	631.71	Joback Method
cpg	418.33	J/mol×K	665.87	Joback Method
cpg	430.83	J/mol×K	700.03	Joback Method
cpg	442.47	J/mol×K	734.20	Joback Method

Sources

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=U376260&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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