1,6-Heptadien-4-ol, chlorodifluoroacetate

Inchi: InChI=1S/C9H11ClF2O2/c1-3-5-7(6-4-2)14-8(13)9(10,11)12/h3-4,7H,1-2,5-6H2
InchiKey: JPRRPDFZSRIYTG-UHFFFAOYSA-N
Formula: C9H11ClF2O2
SMILES: C=CCC(CC=C)OC(=O)C(F)(F)Cl
Mol. weight [g/mol]: 224.63

Physical Properties

Property code	Value	Unit	Source
gf	-434.49	kJ/mol	Joback Method
hf	-645.02	kJ/mol	Joback Method
hfus	18.71	kJ/mol	Joback Method
hvap	44.51	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.882		Crippen Method
mcvol	152.290	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rinpol	1010.00		NIST Webbook
rinpol	1010.00		NIST Webbook
tb	507.27	K	Joback Method
tc	689.99	K	Joback Method
tf	278.35	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.51	J/mol×K	507.27	Joback Method
cpg	347.14	J/mol×K	537.72	Joback Method
cpg	358.12	J/mol×K	568.18	Joback Method
cpg	368.46	J/mol×K	598.63	Joback Method
cpg	378.20	J/mol×K	629.09	Joback Method
cpg	387.37	J/mol×K	659.54	Joback Method
cpg	395.98	J/mol×K	689.99	Joback Method

Sources

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=U376231&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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