L-Valine, N-chlorodifluoroacetyl-, ethyl ester

Inchi: InChI=1S/C9H14ClF2NO3/c1-4-16-7(14)6(5(2)3)13-8(15)9(10,11)12/h5-6H,4H2,1-3H3,(H
InchiKey: PNAMAEDJCCYRLF-UHFFFAOYSA-N
Formula: C9H14ClF2NO3
SMILES: CCOC(=O)C(NC(=O)C(F)(F)Cl)C(C)C
Mol. weight [g/mol]: 257.66

Physical Properties

Property code	Value	Unit	Source
gf	-652.14	kJ/mol	Joback Method
hf	-960.27	kJ/mol	Joback Method
hfus	24.45	kJ/mol	Joback Method
hvap	58.64	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.522		Crippen Method
mcvol	172.440	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rinpol	1269.00		NIST Webbook
rinpol	1269.00		NIST Webbook
tb	617.51	K	Joback Method
tc	806.81	K	Joback Method
tf	369.46	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.04	J/mol×K	617.51	Joback Method
cpg	451.94	J/mol×K	649.06	Joback Method
cpg	463.13	J/mol×K	680.61	Joback Method
cpg	473.64	J/mol×K	712.16	Joback Method
cpg	483.50	J/mol×K	743.71	Joback Method
cpg	492.71	J/mol×K	775.26	Joback Method
cpg	501.32	J/mol×K	806.81	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=U375635&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