L-Isoleucine, N-chlorodifluoroacetyl-, ethyl ester

Inchi: InChI=1S/C10H16ClF2NO3/c1-4-6(3)7(8(15)17-5-2)14-9(16)10(11,12)13/h6-7H,4-5H2,1-

InchiKey: DGWDUKMYXDNFQI-UHFFFAOYSA-N

Formula: C10H16ClF2NO3

SMILES: CCOC(=O)C(NC(=O)C(F)(F)Cl)C(C)CC

Mol. weight [g/mol]: 271.69

Physical Properties

Property code	Value	Unit	Source
gf	-643.72	kJ/mol	Joback Method
hf	-980.91	kJ/mol	Joback Method
hfus	27.04	kJ/mol	Joback Method
hvap	60.87	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	1.912		Crippen Method
mcvol	186.530	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	1351.00		NIST Webbook
rinpol	1351.00		NIST Webbook
tb	640.39	K	Joback Method
tc	827.82	K	Joback Method
tf	380.73	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.48	J/mol×K	640.39	Joback Method
cpg	501.98	J/mol×K	671.63	Joback Method
cpg	513.74	J/mol×K	702.87	Joback Method
cpg	524.79	J/mol×K	734.11	Joback Method
cpg	535.15	J/mol×K	765.34	Joback Method
cpg	544.85	J/mol×K	796.58	Joback Method
cpg	553.92	J/mol×K	827.82	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=U375629&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