D-«alpha»-Cyclohexylglycine, N-chlorodifluoroacetyl-, ethyl ester

Inchi: InChI=1S/C12H18ClF2NO3/c1-2-19-10(17)9(8-6-4-3-5-7-8)16-11(18)12(13,14)15/h8-9H,

InchiKey: OTKQMSIYEJDWKH-UHFFFAOYSA-N

Formula: C12H18ClF2NO3

SMILES: CCOC(=O)C(NC(=O)C(F)(F)Cl)C1CCCCC1

Mol. weight [g/mol]: 297.73

Physical Properties

Property code	Value	Unit	Source
gf	-599.99	kJ/mol	Joback Method
hf	-962.59	kJ/mol	Joback Method
hfus	27.58	kJ/mol	Joback Method
hvap	66.14	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.446		Crippen Method
mcvol	203.850	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1628.00		NIST Webbook
tb	706.14	K	Joback Method
tc	913.46	K	Joback Method
tf	425.65	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.27	J/mol×K	706.14	Joback Method
cpg	599.46	J/mol×K	740.69	Joback Method
cpg	613.55	J/mol×K	775.25	Joback Method
cpg	626.59	J/mol×K	809.80	Joback Method
cpg	638.61	J/mol×K	844.35	Joback Method
cpg	649.66	J/mol×K	878.90	Joback Method
cpg	659.79	J/mol×K	913.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375804&Units=SI
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

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