hydroxyaspartic acid, trifluoroacetyl-isopropyl ester

Inchi: InChI=1S/C14H23NO7/c1-7(2)20-13(18)11(15-9(5)16)12(22-10(6)17)14(19)21-8(3)4/h7-8

InchiKey: ASCXPNFSNANMFN-VXGBXAGGSA-N

Formula: C14H23NO7

SMILES: CC(=O)NC(C(=O)OC(C)C)C(OC(C)=O)C(=O)OC(C)C

Mol. weight [g/mol]: 317.33

Physical Properties

Property code	Value	Unit	Source
gf	-684.05	kJ/mol	Joback Method
hf	-1146.92	kJ/mol	Joback Method
hfus	32.98	kJ/mol	Joback Method
hvap	85.86	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	0.326		Crippen Method
mcvol	241.990	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	1352.00		NIST Webbook
tb	850.87	K	Joback Method
tc	1054.72	K	Joback Method
tf	506.61	K	Joback Method
vc	0.908	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.50	J/mol×K	850.87	Joback Method
cpg	758.07	J/mol×K	884.84	Joback Method
cpg	769.51	J/mol×K	918.82	Joback Method
cpg	779.81	J/mol×K	952.79	Joback Method
cpg	788.97	J/mol×K	986.77	Joback Method
cpg	796.97	J/mol×K	1020.74	Joback Method
cpg	803.81	J/mol×K	1054.72	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=R522526&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