serine, trifluoroacetyl-isopropyl ester

Inchi: InChI=1S/C10H11F6NO5/c1-4(2)22-6(18)5(17-7(19)9(11,12)13)3-21-8(20)10(14,15)16/h
InchiKey: AAADJZHJPLWCSI-UHFFFAOYSA-N
Formula: C10H11F6NO5
SMILES: CC(C)OC(=O)C(COC(=O)C(F)(F)F)NC(=O)C(F)(F)F
Mol. weight [g/mol]: 339.19

Physical Properties

Property code	Value	Unit	Source
gf	-1642.11	kJ/mol	Joback Method
hf	-2003.16	kJ/mol	Joback Method
hfus	30.53	kJ/mol	Joback Method
hvap	61.08	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.091		Crippen Method
mcvol	188.810	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
rinpol	1175.00		NIST Webbook
rinpol	1175.00		NIST Webbook
tb	673.10	K	Joback Method
tc	845.99	K	Joback Method
tf	427.75	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.87	J/mol×K	673.10	Joback Method
cpg	550.29	J/mol×K	701.91	Joback Method
cpg	560.03	J/mol×K	730.73	Joback Method
cpg	569.13	J/mol×K	759.54	Joback Method
cpg	577.59	J/mol×K	788.36	Joback Method
cpg	585.45	J/mol×K	817.17	Joback Method
cpg	592.72	J/mol×K	845.99	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=R267982&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