cysteine, trifluoroacetyl-isopropyl ester

Inchi: InChI=1S/C10H11F6NO4S/c1-4(2)21-6(18)5(17-7(19)9(11,12)13)3-22-8(20)10(14,15)16/
InchiKey: LMJLCJJCFOICOI-UHFFFAOYSA-N
Formula: C10H11F6NO4S
SMILES: CC(C)OC(=O)C(CSC(=O)C(F)(F)F)NC(=O)C(F)(F)F
Mol. weight [g/mol]: 355.25

Physical Properties

Property code	Value	Unit	Source
gf	-1503.99	kJ/mol	Joback Method
hf	-1829.07	kJ/mol	Joback Method
hfus	33.48	kJ/mol	Joback Method
hvap	65.48	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	1.807		Crippen Method
mcvol	199.290	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	1302.00		NIST Webbook
rinpol	1302.00		NIST Webbook
tb	719.46	K	Joback Method
tc	905.91	K	Joback Method
tf	439.92	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.32	J/mol×K	719.46	Joback Method
cpg	575.29	J/mol×K	750.53	Joback Method
cpg	584.51	J/mol×K	781.61	Joback Method
cpg	593.00	J/mol×K	812.68	Joback Method
cpg	600.80	J/mol×K	843.76	Joback Method
cpg	607.94	J/mol×K	874.83	Joback Method
cpg	614.46	J/mol×K	905.91	Joback Method

Sources

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=R267853&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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