methionine, trifluoroacetyl-isopropyl ester

Inchi: InChI=1S/C10H16F3NO3S/c1-6(2)17-8(15)7(4-5-18-3)14-9(16)10(11,12)13/h6-7H,4-5H2
InchiKey: VYXDFEHRYSPREV-UHFFFAOYSA-N
Formula: C10H16F3NO3S
SMILES: CSCCC(NC(=O)C(F)(F)F)C(=O)OC(C)C
Mol. weight [g/mol]: 287.30

Physical Properties

Property code	Value	Unit	Source
gf	-793.48	kJ/mol	Joback Method
hf	-1119.41	kJ/mol	Joback Method
hfus	30.05	kJ/mol	Joback Method
hvap	62.49	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	1.738		Crippen Method
mcvol	192.410	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	1465.00		NIST Webbook
rinpol	1465.00		NIST Webbook
tb	671.01	K	Joback Method
tc	861.79	K	Joback Method
tf	385.80	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.66	J/mol×K	671.01	Joback Method
cpg	537.16	J/mol×K	702.81	Joback Method
cpg	548.87	J/mol×K	734.60	Joback Method
cpg	559.83	J/mol×K	766.40	Joback Method
cpg	570.05	J/mol×K	798.20	Joback Method
cpg	579.55	J/mol×K	829.99	Joback Method
cpg	588.35	J/mol×K	861.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R267942&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

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