l-Methionine, n-pentafluoropropionyl-, ethyl ester

Inchi: InChI=1S/C10H14F5NO3S/c1-3-19-7(17)6(4-5-20-2)16-8(18)9(11,12)10(13,14)15/h6H,3-

InchiKey: BTWCDYIZXWZLDF-UHFFFAOYSA-N

Formula: C10H14F5NO3S

SMILES: CCOC(=O)C(CCSC)NC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 323.28

Physical Properties

Property code	Value	Unit	Source
gf	-1177.82	kJ/mol	Joback Method
hf	-1515.10	kJ/mol	Joback Method
hfus	32.32	kJ/mol	Joback Method
hvap	59.94	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	1.985		Crippen Method
mcvol	195.950	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	1448.00		NIST Webbook
rinpol	1448.00		NIST Webbook
tb	666.76	K	Joback Method
tc	849.28	K	Joback Method
tf	404.40	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.24	J/mol×K	666.76	Joback Method
cpg	554.86	J/mol×K	697.18	Joback Method
cpg	565.73	J/mol×K	727.60	Joback Method
cpg	575.85	J/mol×K	758.02	Joback Method
cpg	585.28	J/mol×K	788.44	Joback Method
cpg	594.04	J/mol×K	818.86	Joback Method
cpg	602.16	J/mol×K	849.28	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=U320909&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