l-Methionine, n-heptafluorobutyryl-, ethyl ester

Inchi: InChI=1S/C11H14F7NO3S/c1-3-22-7(20)6(4-5-23-2)19-8(21)9(12,13)10(14,15)11(16,17)
InchiKey: YACKYESRXIZBCN-UHFFFAOYSA-N
Formula: C11H14F7NO3S
SMILES: CCOC(=O)C(CCSC)NC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 373.29

Physical Properties

Property code	Value	Unit	Source
gf	-1556.18	kJ/mol	Joback Method
hf	-1936.71	kJ/mol	Joback Method
hfus	33.66	kJ/mol	Joback Method
hvap	59.24	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	2.620		Crippen Method
mcvol	213.580	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
rinpol	1471.00		NIST Webbook
tb	684.95	K	Joback Method
tc	862.07	K	Joback Method
tf	419.27	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.50	J/mol×K	684.95	Joback Method
cpg	624.98	J/mol×K	714.47	Joback Method
cpg	635.66	J/mol×K	743.99	Joback Method
cpg	645.59	J/mol×K	773.51	Joback Method
cpg	654.80	J/mol×K	803.03	Joback Method
cpg	663.34	J/mol×K	832.55	Joback Method
cpg	671.26	J/mol×K	862.07	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=U320849&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