l-Methionine, n-pentafluoropropionyl-, undecyl ester

Inchi: InChI=1S/C19H32F5NO3S/c1-3-4-5-6-7-8-9-10-11-13-28-16(26)15(12-14-29-2)25-17(27

InchiKey: YAXAGLAOAOOMCH-UHFFFAOYSA-N

Formula: C19H32F5NO3S

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

Mol. weight [g/mol]: 449.52

Physical Properties

Property code	Value	Unit	Source
gf	-1102.04	kJ/mol	Joback Method
hf	-1700.86	kJ/mol	Joback Method
hfus	55.63	kJ/mol	Joback Method
hvap	79.98	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	5.496		Crippen Method
mcvol	322.760	ml/mol	McGowan Method
pc	1052.77	kPa	Joback Method
rinpol	2279.00		NIST Webbook
rinpol	2279.00		NIST Webbook
tb	872.68	K	Joback Method
tc	1068.49	K	Joback Method
tf	505.83	K	Joback Method
vc	1.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1044.27	J/mol×K	872.68	Joback Method
cpg	1059.61	J/mol×K	905.31	Joback Method
cpg	1073.91	J/mol×K	937.95	Joback Method
cpg	1087.21	J/mol×K	970.58	Joback Method
cpg	1099.58	J/mol×K	1003.22	Joback Method
cpg	1111.09	J/mol×K	1035.85	Joback Method
cpg	1121.79	J/mol×K	1068.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320919&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