l-Methionine, n-pentafluoropropionyl-, nonyl ester

Inchi: InChI=1S/C17H28F5NO3S/c1-3-4-5-6-7-8-9-11-26-14(24)13(10-12-27-2)23-15(25)16(18
InchiKey: XBLRLROWVPYLCX-UHFFFAOYSA-N
Formula: C17H28F5NO3S
SMILES: CCCCCCCCCOC(=O)C(CCSC)NC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 421.47

Physical Properties

Property code	Value	Unit	Source
gf	-1118.88	kJ/mol	Joback Method
hf	-1659.58	kJ/mol	Joback Method
hfus	50.45	kJ/mol	Joback Method
hvap	75.53	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	4.716		Crippen Method
mcvol	294.580	ml/mol	McGowan Method
pc	1197.30	kPa	Joback Method
rinpol	2089.00		NIST Webbook
rinpol	2089.00		NIST Webbook
tb	826.92	K	Joback Method
tc	1014.99	K	Joback Method
tf	483.29	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	926.50	J/mol×K	826.92	Joback Method
cpg	940.98	J/mol×K	858.26	Joback Method
cpg	954.50	J/mol×K	889.61	Joback Method
cpg	967.12	J/mol×K	920.95	Joback Method
cpg	978.87	J/mol×K	952.30	Joback Method
cpg	989.81	J/mol×K	983.64	Joback Method
cpg	1000.00	J/mol×K	1014.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320917&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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