l-Methionine, n-heptafluorobutyryl-, nonyl ester

Inchi: InChI=1S/C18H28F7NO3S/c1-3-4-5-6-7-8-9-11-29-14(27)13(10-12-30-2)26-15(28)16(19

InchiKey: CHOCDBCSBUQJFU-UHFFFAOYSA-N

Formula: C18H28F7NO3S

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

Mol. weight [g/mol]: 471.47

Physical Properties

Property code	Value	Unit	Source
gf	-1497.24	kJ/mol	Joback Method
hf	-2081.19	kJ/mol	Joback Method
hfus	51.79	kJ/mol	Joback Method
hvap	74.82	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	5.351		Crippen Method
mcvol	312.210	ml/mol	McGowan Method
pc	1070.06	kPa	Joback Method
rinpol	2099.00		NIST Webbook
rinpol	2099.00		NIST Webbook
tb	845.11	K	Joback Method
tc	1035.01	K	Joback Method
tf	498.16	K	Joback Method
vc	1.250	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.73	J/mol×K	845.11	Joback Method
cpg	1015.09	J/mol×K	876.76	Joback Method
cpg	1028.48	J/mol×K	908.41	Joback Method
cpg	1040.97	J/mol×K	940.06	Joback Method
cpg	1052.64	J/mol×K	971.71	Joback Method
cpg	1063.55	J/mol×K	1003.36	Joback Method
cpg	1073.77	J/mol×K	1035.01	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=U320856&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