l-Methionine, n-heptafluorobutyryl-, octadecyl ester

Inchi: InChI=1S/C27H46F7NO3S/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-20-38-23(36)2

InchiKey: JCPJZQWZKJKSCL-UHFFFAOYSA-N

Formula: C27H46F7NO3S

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

Mol. weight [g/mol]: 597.71

Physical Properties

Property code	Value	Unit	Source
gf	-1421.46	kJ/mol	Joback Method
hf	-2266.95	kJ/mol	Joback Method
hfus	75.10	kJ/mol	Joback Method
hvap	94.86	kJ/mol	Joback Method
log10ws	-10.24		Crippen Method
logp	8.862		Crippen Method
mcvol	439.020	ml/mol	McGowan Method
pc	650.44	kPa	Joback Method
rinpol	3041.00		NIST Webbook
rinpol	3041.00		NIST Webbook
tb	1051.03	K	Joback Method
tc	1324.82	K	Joback Method
tf	599.59	K	Joback Method
vc	1.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1552.65	J/mol×K	1051.03	Joback Method
cpg	1573.87	J/mol×K	1096.66	Joback Method
cpg	1593.51	J/mol×K	1142.29	Joback Method
cpg	1611.85	J/mol×K	1187.93	Joback Method
cpg	1629.16	J/mol×K	1233.56	Joback Method
cpg	1645.71	J/mol×K	1279.19	Joback Method
cpg	1661.78	J/mol×K	1324.82	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=U320863&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