l-Methionine, n-heptafluorobutyryl-, heptadecyl ester

Inchi: InChI=1S/C26H44F7NO3S/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-19-37-22(35)21(1

InchiKey: DYRIRNRDMTWMNS-UHFFFAOYSA-N

Formula: C26H44F7NO3S

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

Mol. weight [g/mol]: 583.69

Physical Properties

Property code	Value	Unit	Source
gf	-1429.88	kJ/mol	Joback Method
hf	-2246.31	kJ/mol	Joback Method
hfus	72.51	kJ/mol	Joback Method
hvap	92.63	kJ/mol	Joback Method
log10ws	-9.82		Crippen Method
logp	8.472		Crippen Method
mcvol	424.930	ml/mol	McGowan Method
pc	683.50	kPa	Joback Method
rinpol	2892.00		NIST Webbook
rinpol	2892.00		NIST Webbook
tb	1028.15	K	Joback Method
tc	1287.17	K	Joback Method
tf	588.32	K	Joback Method
vc	1.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1489.15	J/mol×K	1028.15	Joback Method
cpg	1509.24	J/mol×K	1071.32	Joback Method
cpg	1527.84	J/mol×K	1114.49	Joback Method
cpg	1545.19	J/mol×K	1157.66	Joback Method
cpg	1561.51	J/mol×K	1200.83	Joback Method
cpg	1577.01	J/mol×K	1244.00	Joback Method
cpg	1591.93	J/mol×K	1287.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320862&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