l-Methionine, n-pentafluoropropionyl-, hexadecyl ester

Inchi: InChI=1S/C24H42F5NO3S/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-18-33-21(31)20(17-1

InchiKey: UGPZSFRLBSETOP-UHFFFAOYSA-N

Formula: C24H42F5NO3S

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

Mol. weight [g/mol]: 519.65

Physical Properties

Property code	Value	Unit	Source
gf	-1059.94	kJ/mol	Joback Method
hf	-1804.06	kJ/mol	Joback Method
hfus	68.58	kJ/mol	Joback Method
hvap	91.11	kJ/mol	Joback Method
log10ws	-8.67		Crippen Method
logp	7.446		Crippen Method
mcvol	393.210	ml/mol	McGowan Method
pc	788.16	kPa	Joback Method
rinpol	2783.00		NIST Webbook
rinpol	2783.00		NIST Webbook
tb	987.08	K	Joback Method
tc	1219.64	K	Joback Method
tf	562.18	K	Joback Method
vc	1.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1350.10	J/mol×K	987.08	Joback Method
cpg	1368.37	J/mol×K	1025.84	Joback Method
cpg	1385.21	J/mol×K	1064.60	Joback Method
cpg	1400.74	J/mol×K	1103.36	Joback Method
cpg	1415.10	J/mol×K	1142.12	Joback Method
cpg	1428.39	J/mol×K	1180.88	Joback Method
cpg	1440.76	J/mol×K	1219.64	Joback Method

Sources

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=U320923&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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