l-Methionine, n-heptafluorobutyryl-, pentadecyl ester

Inchi: InChI=1S/C24H40F7NO3S/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-17-35-20(33)19(16-18-3

InchiKey: DGPJRLNCMSOIIK-UHFFFAOYSA-N

Formula: C24H40F7NO3S

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

Mol. weight [g/mol]: 555.63

Physical Properties

Property code	Value	Unit	Source
gf	-1446.72	kJ/mol	Joback Method
hf	-2205.03	kJ/mol	Joback Method
hfus	67.33	kJ/mol	Joback Method
hvap	88.18	kJ/mol	Joback Method
log10ws	-8.98		Crippen Method
logp	7.692		Crippen Method
mcvol	396.750	ml/mol	McGowan Method
pc	757.65	kPa	Joback Method
rinpol	2660.00		NIST Webbook
rinpol	2660.00		NIST Webbook
tb	982.39	K	Joback Method
tc	1216.59	K	Joback Method
tf	565.78	K	Joback Method
vc	1.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1363.59	J/mol×K	982.39	Joback Method
cpg	1381.77	J/mol×K	1021.42	Joback Method
cpg	1398.63	J/mol×K	1060.46	Joback Method
cpg	1414.34	J/mol×K	1099.49	Joback Method
cpg	1429.05	J/mol×K	1138.52	Joback Method
cpg	1442.91	J/mol×K	1177.56	Joback Method
cpg	1456.09	J/mol×K	1216.59	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=U320861&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