l-Methionine, n-heptafluorobutyryl-, tetradecyl ester

Inchi: InChI=1S/C23H38F7NO3S/c1-3-4-5-6-7-8-9-10-11-12-13-14-16-34-19(32)18(15-17-35-2
InchiKey: YQPKMJSNXAVJSX-UHFFFAOYSA-N
Formula: C23H38F7NO3S
SMILES: CCCCCCCCCCCCCCOC(=O)C(CCSC)NC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 541.61

Physical Properties

Property code	Value	Unit	Source
gf	-1455.14	kJ/mol	Joback Method
hf	-2184.39	kJ/mol	Joback Method
hfus	64.74	kJ/mol	Joback Method
hvap	85.95	kJ/mol	Joback Method
log10ws	-8.56		Crippen Method
logp	7.302		Crippen Method
mcvol	382.660	ml/mol	McGowan Method
pc	799.34	kPa	Joback Method
rinpol	2455.00		NIST Webbook
tb	959.51	K	Joback Method
tc	1183.43	K	Joback Method
tf	554.51	K	Joback Method
vc	1.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1301.60	J/mol×K	959.51	Joback Method
cpg	1318.96	J/mol×K	996.83	Joback Method
cpg	1335.09	J/mol×K	1034.15	Joback Method
cpg	1350.11	J/mol×K	1071.47	Joback Method
cpg	1364.16	J/mol×K	1108.79	Joback Method
cpg	1377.38	J/mol×K	1146.11	Joback Method
cpg	1389.88	J/mol×K	1183.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320860&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

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