l-Methionine, n-pentafluoropropionyl-, pentadecyl ester

Inchi: InChI=1S/C23H40F5NO3S/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-17-32-20(30)19(16-18-3

InchiKey: XSCFPCVGWDCWRC-UHFFFAOYSA-N

Formula: C23H40F5NO3S

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

Mol. weight [g/mol]: 505.63

Physical Properties

Property code	Value	Unit	Source
gf	-1068.36	kJ/mol	Joback Method
hf	-1783.42	kJ/mol	Joback Method
hfus	65.99	kJ/mol	Joback Method
hvap	88.88	kJ/mol	Joback Method
log10ws	-8.25		Crippen Method
logp	7.056		Crippen Method
mcvol	379.120	ml/mol	McGowan Method
pc	832.42	kPa	Joback Method
rinpol	2671.00		NIST Webbook
tb	964.20	K	Joback Method
tc	1187.09	K	Joback Method
tf	550.91	K	Joback Method
vc	1.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1287.81	J/mol×K	964.20	Joback Method
cpg	1305.38	J/mol×K	1001.35	Joback Method
cpg	1321.61	J/mol×K	1038.50	Joback Method
cpg	1336.62	J/mol×K	1075.65	Joback Method
cpg	1350.50	J/mol×K	1112.80	Joback Method
cpg	1363.37	J/mol×K	1149.94	Joback Method
cpg	1375.32	J/mol×K	1187.09	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=U320922&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

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