l-Methionine, n-pentafluoropropionyl-, tetradecyl ester

Inchi: InChI=1S/C22H38F5NO3S/c1-3-4-5-6-7-8-9-10-11-12-13-14-16-31-19(29)18(15-17-32-2
InchiKey: DTTUCZXPUVFDOO-UHFFFAOYSA-N
Formula: C22H38F5NO3S
SMILES: CCCCCCCCCCCCCCOC(=O)C(CCSC)NC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 491.60

Physical Properties

Property code	Value	Unit	Source
gf	-1076.78	kJ/mol	Joback Method
hf	-1762.78	kJ/mol	Joback Method
hfus	63.40	kJ/mol	Joback Method
hvap	86.66	kJ/mol	Joback Method
log10ws	-7.83		Crippen Method
logp	6.666		Crippen Method
mcvol	365.030	ml/mol	McGowan Method
pc	880.52	kPa	Joback Method
rinpol	2569.00		NIST Webbook
rinpol	2569.00		NIST Webbook
tb	941.32	K	Joback Method
tc	1155.80	K	Joback Method
tf	539.64	K	Joback Method
vc	1.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1226.04	J/mol×K	941.32	Joback Method
cpg	1242.98	J/mol×K	977.07	Joback Method
cpg	1258.66	J/mol×K	1012.81	Joback Method
cpg	1273.18	J/mol×K	1048.56	Joback Method
cpg	1286.64	J/mol×K	1084.30	Joback Method
cpg	1299.12	J/mol×K	1120.05	Joback Method
cpg	1310.72	J/mol×K	1155.80	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=U320921&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