l-Methionine, n-pentafluoropropionyl-, hexyl ester

Inchi: InChI=1S/C14H22F5NO3S/c1-3-4-5-6-8-23-11(21)10(7-9-24-2)20-12(22)13(15,16)14(17

InchiKey: WZLUIWQFKXPIIW-UHFFFAOYSA-N

Formula: C14H22F5NO3S

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

Mol. weight [g/mol]: 379.39

Physical Properties

Property code	Value	Unit	Source
gf	-1144.14	kJ/mol	Joback Method
hf	-1597.66	kJ/mol	Joback Method
hfus	42.68	kJ/mol	Joback Method
hvap	68.85	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.545		Crippen Method
mcvol	252.310	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
rinpol	1796.00		NIST Webbook
tb	758.28	K	Joback Method
tc	940.44	K	Joback Method
tf	449.48	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.08	J/mol×K	758.28	Joback Method
cpg	769.40	J/mol×K	788.64	Joback Method
cpg	781.85	J/mol×K	819.00	Joback Method
cpg	793.49	J/mol×K	849.36	Joback Method
cpg	804.34	J/mol×K	879.72	Joback Method
cpg	814.46	J/mol×K	910.08	Joback Method
cpg	823.87	J/mol×K	940.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320914&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