l-Methionine, n-pentafluoropropionyl-, heptyl ester

Inchi: InChI=1S/C15H24F5NO3S/c1-3-4-5-6-7-9-24-12(22)11(8-10-25-2)21-13(23)14(16,17)15

InchiKey: KLWDJOCSFZRADF-UHFFFAOYSA-N

Formula: C15H24F5NO3S

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

Mol. weight [g/mol]: 393.41

Physical Properties

Property code	Value	Unit	Source
gf	-1135.72	kJ/mol	Joback Method
hf	-1618.30	kJ/mol	Joback Method
hfus	45.27	kJ/mol	Joback Method
hvap	71.07	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.935		Crippen Method
mcvol	266.400	ml/mol	McGowan Method
pc	1373.78	kPa	Joback Method
rinpol	1897.00		NIST Webbook
rinpol	1897.00		NIST Webbook
tb	781.16	K	Joback Method
tc	964.61	K	Joback Method
tf	460.75	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.98	J/mol×K	781.16	Joback Method
cpg	825.68	J/mol×K	811.74	Joback Method
cpg	838.48	J/mol×K	842.31	Joback Method
cpg	850.45	J/mol×K	872.89	Joback Method
cpg	861.60	J/mol×K	903.46	Joback Method
cpg	872.00	J/mol×K	934.04	Joback Method
cpg	881.68	J/mol×K	964.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320915&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