l-Methionine, n-pentafluoropropionyl-, octyl ester

Inchi: InChI=1S/C16H26F5NO3S/c1-3-4-5-6-7-8-10-25-13(23)12(9-11-26-2)22-14(24)15(17,18)16(19,20)21/h12H,3-11H2,1-2H3,(H,22,24)/t12-/m0/s1

InchiKey: XQLOQVWYMYTKAS-UHFFFAOYSA-N

Formula: C16H26F5NO3S

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

Mol. weight [g/mol]: 407.44

Physical Properties

Property code	Value	Unit	Source
gf	-1127.30	kJ/mol	Joback Method
hf	-1638.94	kJ/mol	Joback Method
hfus	47.86	kJ/mol	Joback Method
hvap	73.30	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.326		Crippen Method
mcvol	280.490	ml/mol	McGowan Method
pc	1280.99	kPa	Joback Method
rinpol	1983.00		NIST Webbook
tb	804.04	K	Joback Method
tc	989.44	K	Joback Method
tf	472.02	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	868.81	J/mol×K	804.04	Joback Method
cpg	882.89	J/mol×K	834.94	Joback Method
cpg	896.05	J/mol×K	865.84	Joback Method
cpg	908.33	J/mol×K	896.74	Joback Method
cpg	919.79	J/mol×K	927.64	Joback Method
cpg	930.46	J/mol×K	958.54	Joback Method
cpg	940.40	J/mol×K	989.44	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320916&Units=SI

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