l-Methionine, n-pentafluoropropionyl-, decyl ester

Inchi: InChI=1S/C18H30F5NO3S/c1-3-4-5-6-7-8-9-10-12-27-15(25)14(11-13-28-2)24-16(26)17

InchiKey: IARFMHZEUTYHEI-UHFFFAOYSA-N

Formula: C18H30F5NO3S

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

Mol. weight [g/mol]: 435.49

Physical Properties

Property code	Value	Unit	Source
gf	-1110.46	kJ/mol	Joback Method
hf	-1680.22	kJ/mol	Joback Method
hfus	53.04	kJ/mol	Joback Method
hvap	77.75	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.106		Crippen Method
mcvol	308.670	ml/mol	McGowan Method
pc	1121.55	kPa	Joback Method
rinpol	2180.00		NIST Webbook
tb	849.80	K	Joback Method
tc	1041.32	K	Joback Method
tf	494.56	K	Joback Method
vc	1.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	985.01	J/mol×K	849.80	Joback Method
cpg	999.91	J/mol×K	881.72	Joback Method
cpg	1013.80	J/mol×K	913.64	Joback Method
cpg	1026.75	J/mol×K	945.56	Joback Method
cpg	1038.81	J/mol×K	977.48	Joback Method
cpg	1050.03	J/mol×K	1009.40	Joback Method
cpg	1060.47	J/mol×K	1041.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320918&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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