L-Methionine, N-pentafluoropropionyl-, dodecyl ester

Inchi: InChI=1S/C20H34F5NO3S/c1-3-4-5-6-7-8-9-10-11-12-14-29-17(27)16(13-15-30-2)26-18

InchiKey: MPJHLDRVTBZNEK-UHFFFAOYSA-N

Formula: C20H34F5NO3S

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

Mol. weight [g/mol]: 463.55

Physical Properties

Property code	Value	Unit	Source
hfus	58.22	kJ/mol	Joback Method
logp	5.886		Crippen Method
mcvol	336.850	ml/mol	McGowan Method
rinpol	2378.00		NIST Webbook
rinpol	2378.00		NIST Webbook
tb	617.87	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1104.23	J/mol×K	895.56	Joback Method
cpg	1120.05	J/mol×K	929.06	Joback Method
cpg	1134.77	J/mol×K	962.57	Joback Method
cpg	1148.45	J/mol×K	996.07	Joback Method
cpg	1161.16	J/mol×K	1029.57	Joback Method
cpg	1172.97	J/mol×K	1063.07	Joback Method
cpg	1183.95	J/mol×K	1096.58	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320920&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature