

L-Methionine, N-pentafluoropropionyl-, nonyl ester

Inchi:	InChI=1S/C17H28F5NO3S/c1-3-4-5-6-7-8-9-11-26-14(24)13(10-12-27-2)23-15(25)16(18)
InchiKey:	XBLRLROWVPYLCX-UHFFFAOYSA-N
Formula:	C17H28F5NO3S
SMILES:	CCCCCCCCCOC(=O)C(CCSC)NC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	421.47

Physical Properties

Property code	Value	Unit	Source
hfus	50.45	kJ/mol	Joback Method
logp	4.716		Crippen Method
mcvol	294.580	ml/mol	McGowan Method
rinpol	2089.00		NIST Webbook
rinpol	2089.00		NIST Webbook
tb	589.97	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	926.50	J/mol×K	826.92	Joback Method
cpg	940.98	J/mol×K	858.26	Joback Method
cpg	954.50	J/mol×K	889.61	Joback Method
cpg	967.12	J/mol×K	920.95	Joback Method
cpg	978.87	J/mol×K	952.30	Joback Method
cpg	989.81	J/mol×K	983.64	Joback Method
cpg	1000.00	J/mol×K	1014.99	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U320917&Units=SI>

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

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

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