

(E)-10-Dodecenoic acid, 9,12-dioxo, methyl ester, bis-PFB-oxime, # 2

Inchi: InChI=1S/C27H24F10N2O4/c1-41-17(40)10-6-4-2-3-5-8-14(39-43-13-16-20(30)24(34)27
InchiKey: ZGSYEMOJGIYNMK-HUXKIHLSA-N
Formula: C27H24F10N2O4
SMILES: COC(=O)CCCCCCC(C=CC=NOCc1c(F)c(F)c(F)c(F)c1F)=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 630.47

Physical Properties

Property code	Value	Unit	Source
hf	-2440.72	kJ/mol	Joback Method
hvap	99.34	kJ/mol	Joback Method
log10ws	-10.84		Crippen Method
logp	7.613		Crippen Method
mcvol	387.710	ml/mol	McGowan Method
pc	661.19	kPa	Joback Method
rinpol	3085.00		NIST Webbook
tb	1191.55	K	Joback Method
tc	1515.01	K	Joback Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R554919&Units=SI>

Legend

hf: Enthalpy of formation 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

Latest version available from:

<https://www.cheméo.com/cid/70-301-9/E-10-Dodecenoic-acid-9-12-dioxo-methyl-ester-bis-PFB-oxime-2.pdf>

Generated by Cheméo on 2024-04-19 18:33:35.457121975 +0000 UTC m=+15840864.377699286.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.