

10,12-Octadecadienoic acid, 9-oxo, PFBO, methyl ester, # 1

Inchi: InChI=1S/C26H34F5NO3/c1-3-4-5-6-7-9-12-15-19(16-13-10-8-11-14-17-21(33)34-2)32-3
InchiKey: JKBVZIAOZGHJMV-STKYPROPSA-N
Formula: C26H34F5NO3
SMILES: CCCCCC=CC=CC(CCCCCCCC(=O)OC)=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 503.55

Physical Properties

Property code	Value	Unit	Source
hf	-1451.49	kJ/mol	Joback Method
hvap	89.85	kJ/mol	Joback Method
log10ws	-9.77		Crippen Method
logp	7.851		Crippen Method
mcvol	372.680	ml/mol	McGowan Method
pc	750.61	kPa	Joback Method
rinpol	2798.00		NIST Webbook
rinpol	2806.00		NIST Webbook
rinpol	2798.00		NIST Webbook
tb	1025.80	K	Joback Method
tc	1264.39	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=R398724&Units=SI>

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

Latest version available from:

<https://www.cheméo.com/cid/40-677-6/10-12-Octadecadienoic-acid-9-oxo-PFBO-methyl-ester-1.pdf>

Generated by Cheméo on 2024-05-01 19:14:49.121214113 +0000 UTC m=+16880138.041791429.

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