Sarcosine, n-(2-thienylcarbonyl)-, dodecyl ester

Inchi: InChI=1S/C20H33NO3S/c1-3-4-5-6-7-8-9-10-11-12-15-24-19(22)17-21(2)20(23)18-14-13

InchiKey: YTZFISPKTNLFTG-UHFFFAOYSA-N

Formula: C20H33NO3S

SMILES: CCCCCCCCCCCCOC(=O)CN(C)C(=O)c1cccs1

Mol. weight [g/mol]: 367.55

Physical Properties

Property code	Value	Unit	Source
hvap	109.15	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.53		Cheméo Relay (1.0)
logp	5.284		Crippen Method
mcvol	308.540	ml/mol	McGowan Method
pc	1213.75	kPa	Cheméo Relay (1.0, beta)
rinpol	2917.00		NIST Webbook
rinpol	2917.00		NIST Webbook
tb	656.05	K	Cheméo Relay (1.0)
tf	313.98	K	Cheméo Relay (1.0)

Sources

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=U321473&Units=SI

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

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

Legend

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
tf:	Normal melting (fusion) point