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

Inchi: InChI=1S/C14H21NO3S/c1-3-4-5-6-9-18-13(16)11-15(2)14(17)12-8-7-10-19-12/h7-8,10H
InchiKey: KFTABTAOBFCDPO-UHFFFAOYSA-N
Formula: C14H21NO3S
SMILES: CCCCCCOC(=O)CN(C)C(=O)c1cccs1
Mol. weight [g/mol]: 283.39

Physical Properties

Property code	Value	Unit	Source
hvap	86.54	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.44		Cheméo Relay (1.0)
logp	2.944		Crippen Method
mcvol	224.000	ml/mol	McGowan Method
pc	1822.31	kPa	Cheméo Relay (1.0, beta)
rinpol	2228.00		NIST Webbook
tb	613.95	K	Cheméo Relay (1.0)
tf	294.18	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321467&Units=SI
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):

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