

1,3-Di-(10-carbethoxydecyl) urea

Inchi: InChI=1S/C27H52N2O5/c1-3-33-25(30)21-17-13-9-5-7-11-15-19-23-28-27(32)29-24-20-
InchiKey: APDVHPWUNQTZIL-UHFFFAOYSA-N
Formula: C27H52N2O5
SMILES: CCOC(=O)CCCCCCCCCN=C(O)NCCCCCCCCCCC(=O)OCC
Mol. weight [g/mol]: 484.71
CAS: 116529-38-5

Physical Properties

Property code	Value	Unit	Source
hf	-1116.54	kJ/mol	Joback Method
hvap	120.52	kJ/mol	Joback Method
log10ws	-7.52		Crippen Method
logp	6.638		Crippen Method
mvol	427.700	ml/mol	McGowan Method
pc	725.35	kPa	Joback Method
tb	1188.65	K	Joback Method
tc	1539.89	K	Joback Method

Sources

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=C116529385&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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