

INTITIETWURKF-UFFFAUTSA-N

Formula: C₃₀H₅₇NO₄

SMILES: CCCCCCCCCCCCCCOC(=O)C(N=C(O)OCC(CC)CCCC)C1CCCCC1

Mol. weight [g/mol]: 495.78

Physical Properties

Property code	Value	Unit	Source
hf	-1075.59	kJ/mol	Joback Method
hvap	113.67	kJ/mol	Joback Method
log10ws	-9.33		Crippen Method
logp	8.937		Crippen Method
mcvol	447.560	ml/mol	McGowan Method
pc	672.55	kPa	Joback Method
tb	1171.92	K	Joback Method
tc	1480.58	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=U383156&Units=SI>

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

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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<https://www.chemeo.com/cid/97-184-1/Glycine-2-cyclohexyl-N-2-ethylhexyl-oxycarbonyl-tridecyl-ester.pdf>

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