

Glycine, 2-cyclohexyl-N-ethoxycarbonyl-, pentadecyl ester

Inchi:	InChI=1S/C26H49NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-19-22-31-25(28)24(27-26(29)3
InchiKey:	MTOXGDBELOKYLL-UHFFFAOYSA-N
Formula:	C26H49NO4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(N=C(O)OCC)C1CCCCC1
Mol. weight [g/mol]:	439.67

Physical Properties

Property code	Value	Unit	Source
hf	-987.75	kJ/mol	Joback Method
hvap	105.15	kJ/mol	Joback Method
log10ws	-7.90		Crippen Method
logp	7.520		Crippen Method
mcvol	391.200	ml/mol	McGowan Method
pc	825.74	kPa	Joback Method
rinpol	3015.00		NIST Webbook
rinpol	3015.00		NIST Webbook
tb	1080.84	K	Joback Method
tc	1336.71	K	Joback Method

Sources

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=U383091&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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