

Carbonic acid, monoamide, N-tetradecyl-, octyl ester

Inchi: InChI=1S/C23H47NO2/c1-3-5-7-9-11-12-13-14-15-16-17-19-21-24-23(25)26-22-20-18-10
InchiKey: VXJSRFAYKWKNJK-UHFFFAOYSA-N
Formula: C23H47NO2
SMILES: CCCCCCCCCCCCCCN=C(O)CCCCCCCC
Mol. weight [g/mol]: 369.62

Physical Properties

Property code	Value	Unit	Source
hf	-730.07	kJ/mol	Joback Method
hvap	89.27	kJ/mol	Joback Method
log10ws	-8.02		Crippen Method
logp	7.979		Crippen Method
mcvol	352.350	ml/mol	McGowan Method
pc	839.67	kPa	Joback Method
rinpol	2726.00		NIST Webbook
rinpol	2726.00		NIST Webbook
tb	916.80	K	Joback Method
tc	1126.12	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=U406922&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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