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

Inchi: InChI=1S/C25H51NO2/c1-3-5-7-9-11-13-14-15-16-17-19-21-23-26-25(27)28-24-22-20-18

InchiKey: JJACPOXTCKVUMI-UHFFFAOYSA-N

Formula: C25H51NO2

SMILES: CCCCCCCCCCCCCCN=C(O)OCCCCCCCCCC

Mol. weight [g/mol]: 397.68

Physical Properties

Property code	Value	Unit	Source
hf	-771.35	kJ/mol	Joback Method
hvap	93.73	kJ/mol	Joback Method
log10ws	-8.85		Crippen Method
logp	8.759		Crippen Method
mcvol	380.530	ml/mol	McGowan Method
pc	753.50	kPa	Joback Method
rinpol	3261.00		NIST Webbook
rinpol	3261.00		NIST Webbook
tb	962.56	K	Joback Method
tc	1190.14	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=U415188&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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