

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

Inchi: InChI=1S/C21H43NO2/c1-3-5-7-9-11-13-15-17-19-22-21(23)24-20-18-16-14-12-10-8-6-4
InchiKey: YCAGETBDIRRFLA-UHFFFAOYSA-N
Formula: C21H43NO2
SMILES: CCCCCCCCCCN=C(O)CCCCCCCCCCC
Mol. weight [g/mol]: 341.57

Physical Properties

Property code	Value	Unit	Source
hf	-688.79	kJ/mol	Joback Method
hvap	84.82	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	7.198		Crippen Method
mcvol	324.170	ml/mol	McGowan Method
pc	941.52	kPa	Joback Method
rinpol	2723.00		NIST Webbook
rinpol	2723.00		NIST Webbook
tb	871.04	K	Joback Method
tc	1066.65	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U415185&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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>

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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