

N-(3-Methoxy)Benzylinooleamide

Inchi:	InChI=1S/C26H41NO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-26(28)27-23-24-19
InchiKey:	BMQBTHWVNBJS-PS-NQLNTRDSA-N
Formula:	C26H41NO2
SMILES:	CCCCC=CCC=CCCCCCCC(O)=NCc1cccc(OC)c1
Mol. weight [g/mol]:	399.61
CAS:	883715-22-8

Physical Properties

Property code	Value	Unit	Source
hf	-332.49	kJ/mol	Joback Method
hvap	98.81	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	7.965		Crippen Method
mvol	362.260	ml/mol	McGowan Method
pc	907.79	kPa	Joback Method
rinpol	3293.40		NIST Webbook
tb	1025.42	K	Joback Method
tc	1257.03	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=C883715228&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

Latest version available from:

<https://www.cheméo.com/cid/86-571-3/N-3-Methoxy-Benzylinoamide.pdf>

Generated by Cheméo on 2024-04-27 08:46:32.42077979 +0000 UTC m=+16496841.341357111.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.