(2E,4E,12E)-N-Isobutyloctadeca-2,4,12-trienamide

Inchi: InChI=1S/C22H39NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22(24)23-20-21(2)
InchiKey: PCWWIOUZYOPZHT-WMVGRUGPSA-N
Formula: C22H39NO
SMILES: CCCCCC=CCCCCCCC=CC=CC(O)=NCC(C)C
Mol. weight [g/mol]: 333.55
CAS: 943546-17-6

Physical Properties

Property code	Value	Unit	Source
hf	-230.83	kJ/mol	Joback Method
hvap	84.12	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	7.188		Crippen Method
mcvol	319.490	ml/mol	McGowan Method
pc	992.63	kPa	Joback Method
rinpol	2776.30		NIST Webbook
rinpol	2776.30		NIST Webbook
tb	883.54	K	Joback Method
tc	1082.68	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C943546176&Units=SI

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