(2E,4E)-N-Isobutyltetradeca-2,4-dienamide

Inchi: InChI=1S/C18H33NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-18(20)19-16-17(2)3/h12-15,17H
InchiKey: AGJAUFUNZWHLKE-SQIWNDBBSA-N
Formula: C18H33NO
SMILES: CCCCCCCCCC=CC=CC(O)=NCC(C)C
Mol. weight [g/mol]: 279.46
CAS: 13891-73-1

Physical Properties

Property code	Value	Unit	Source
hf	-265.49	kJ/mol	Joback Method
hvap	75.26	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.852		Crippen Method
mcvol	267.430	ml/mol	McGowan Method
pc	1238.09	kPa	Joback Method
rinpol	2363.00		NIST Webbook
rinpol	2363.00		NIST Webbook
tb	787.86	K	Joback Method
tc	974.40	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=C13891731&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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