

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

Inchi: InChI=1S/C20H37NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20(22)21-18-19(2)3/h14-
InchiKey: DVBUHWFEXOSULX-JLXBFWJWSA-N
Formula: C20H37NO
SMILES: CCCCCCCCCC=CC=CC(O)=NCC(C)C
Mol. weight [g/mol]: 307.51
CAS: 54794-69-3

Physical Properties

Property code	Value	Unit	Source
hf	-306.77	kJ/mol	Joback Method
hvap	79.71	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	6.632		Crippen Method
mcvol	295.610	ml/mol	McGowan Method
pc	1086.35	kPa	Joback Method
rinpol	2573.10		NIST Webbook
rinpol	2573.10		NIST Webbook
tb	833.62	K	Joback Method
tc	1024.11	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C54794693&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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