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

Inchi: InChI=1S/C12H21NO/c1-4-5-6-7-8-9-12(14)13-10-11(2)3/h6-9,11H,4-5,10H2,1-3H3,(H,1
InchiKey: VZASTVPVPUAAJK-BLHCBFLLSA-N
Formula: C12H21NO
SMILES: CCCC=CC=CC(O)=NCC(C)C
Mol. weight [g/mol]: 195.30
CAS: 23512-47-2

Physical Properties

Property code	Value	Unit	Source
hf	-141.65	kJ/mol	Joback Method
hvap	61.91	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.511		Crippen Method
mcvol	182.890	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	1717.60		NIST Webbook
rinpol	1717.60		NIST Webbook
tb	650.58	K	Joback Method
tc	839.34	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=C23512472&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