

4-n-Pentanoyl-4-n'-dodecanoyloxyazobenzene

Inchi: InChI=1S/C29H40N2O3/c1-3-5-7-8-9-10-11-12-13-15-29(33)34-27-22-20-26(21-23-27)3
InchiKey: KLQXBRFBSNFUKA-NVQSTNCTSA-N
Formula: C29H40N2O3
SMILES: CCCCCCCCCC(=O)Oc1ccc(N=Nc2ccc(C(=O)CCCC)cc2)cc1
Mol. weight [g/mol]: 464.64
CAS: 120103-05-1

Physical Properties

Property code	Value	Unit	Source
hf	-501.93	kJ/mol	Joback Method
hvap	108.60	kJ/mol	Joback Method
log10ws	-9.93		Crippen Method
logp	9.301		Crippen Method
mvol	396.620	ml/mol	McGowan Method
pc	805.70	kPa	Joback Method
tb	1205.60	K	Joback Method
tc	1482.10	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C120103051&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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