

N-(2-Phenylethyl)(2E,6Z,8E)-decatrienamide

Inchi:	InChI=1S/C18H23NO/c1-2-3-4-5-6-7-11-14-18(20)19-16-15-17-12-9-8-10-13-17/h2-5,8-1
InchiKey:	ZVLFTTDBSQNTOB-RSQSAPEFSA-N
Formula:	C18H23NO
SMILES:	CC=CC=CCCC=CC(=O)NCCc1ccccc1
Mol. weight [g/mol]:	269.38

Physical Properties

Property code	Value	Unit	Source
gf	414.22	kJ/mol	Joback Method
hf	114.23	kJ/mol	Joback Method
hfus	43.72	kJ/mol	Joback Method
hvap	70.99	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.814		Crippen Method
mvol	239.370	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	2006.00		NIST Webbook
rinpol	2006.00		NIST Webbook
tb	754.44	K	Joback Method
tc	967.59	K	Joback Method
tf	406.39	K	Joback Method
vc	0.916	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.45	J/mol×K	754.44	Joback Method
cpg	685.47	J/mol×K	789.96	Joback Method
cpg	700.51	J/mol×K	825.49	Joback Method
cpg	714.68	J/mol×K	861.01	Joback Method
cpg	728.07	J/mol×K	896.54	Joback Method
cpg	740.79	J/mol×K	932.06	Joback Method
cpg	752.94	J/mol×K	967.59	Joback Method

Sources

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=U106161&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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