

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:	C/C=C/C=C\C/C=C/C(=O)NCCc1ccccc1
Mol. weight [g/mol]:	269.39

Physical Properties

Property code	Value	Unit	Source
hfus	43.72	kJ/mol	Joback Method
logp	3.814		Crippen Method
mcvol	239.370	ml/mol	McGowan 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

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U106161&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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