

Propanamide, N-tetrahydrofurfuryl-3-phenyl-

Inchi:	InChI=1S/C14H19NO2/c16-14(15-11-13-7-4-10-17-13)9-8-12-5-2-1-3-6-12/h1-3,5-6,13H
InchiKey:	VFWBIIGUCYAVDO-UHFFFAOYSA-N
Formula:	C14H19NO2
SMILES:	O=C(CCc1ccccc1)NCC1CCCO1
Mol. weight [g/mol]:	233.31

Physical Properties

Property code	Value	Unit	Source
gf	90.31	kJ/mol	Joback Method
hf	-226.39	kJ/mol	Joback Method
hfus	34.67	kJ/mol	Joback Method
hvap	66.98	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	1.914		Crippen Method
mvol	190.920	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
rinpol	2003.00		NIST Webbook
rinpol	2003.00		NIST Webbook
tb	692.67	K	Joback Method
tc	918.90	K	Joback Method
tf	414.02	K	Joback Method
vc	0.715	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.09	J/molxK	692.67	Joback Method
cpg	561.33	J/molxK	730.37	Joback Method
cpg	577.30	J/molxK	768.08	Joback Method
cpg	592.08	J/molxK	805.78	Joback Method
cpg	605.72	J/molxK	843.49	Joback Method
cpg	618.31	J/molxK	881.19	Joback Method
cpg	629.90	J/molxK	918.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=U308113&Units=SI

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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