

Propanamide, 3-phenyl-N-ethyl-N-propyl-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C14H21NO/c1-3-12-15(4-2)14(16)11-10-13-8-6-5-7-9-13/h5-9H,3-4,10-12H2,1

AGCSHYFZNTXKDR-UHFFFAOYSA-N

C14H21NO

CCCN(CC)C(=O)CCc1ccccc1

219.32

Physical Properties

Property code	Value	Unit	Source
gf	161.27	kJ/mol	Joback Method
hf	-140.81	kJ/mol	Joback Method
hfus	30.68	kJ/mol	Joback Method
hvap	57.82	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.878		Crippen Method
mcvol	195.910	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinpol	1969.00		NIST Webbook
rinpol	1969.00		NIST Webbook
tb	612.71	K	Joback Method
tc	812.07	K	Joback Method
tf	356.36	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.79	J/mol×K	612.71	Joback Method
cpg	521.85	J/mol×K	645.94	Joback Method
cpg	537.90	J/mol×K	679.16	Joback Method
cpg	552.98	J/mol×K	712.39	Joback Method
cpg	567.15	J/mol×K	745.62	Joback Method
cpg	580.45	J/mol×K	778.84	Joback Method
cpg	592.92	J/mol×K	812.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415390&Units=SI
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

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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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