Propanamide, 3-phenyl-N-ethyl-N-pentyl-

Inchi: InChI=1S/C16H25NO/c1-3-5-9-14-17(4-2)16(18)13-12-15-10-7-6-8-11-15/h6-8,10-11H,3-
InchiKey: WNILCECIJFRFFH-UHFFFAOYSA-N
Formula: C16H25NO
SMILES: CCCCCN(CC)C(=O)CCc1ccccc1
Mol. weight [g/mol]: 247.38

Physical Properties

Property code	Value	Unit	Source
gf	178.11	kJ/mol	Joback Method
hf	-182.09	kJ/mol	Joback Method
hfus	35.86	kJ/mol	Joback Method
hvap	62.28	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.658		Crippen Method
mcvol	224.090	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	2083.00		NIST Webbook
rinpol	2083.00		NIST Webbook
tb	658.47	K	Joback Method
tc	853.00	K	Joback Method
tf	378.90	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.93	J/mol×K	658.47	Joback Method
cpg	628.70	J/mol×K	690.89	Joback Method
cpg	645.44	J/mol×K	723.31	Joback Method
cpg	661.20	J/mol×K	755.73	Joback Method
cpg	676.02	J/mol×K	788.16	Joback Method
cpg	689.97	J/mol×K	820.58	Joback Method
cpg	703.07	J/mol×K	853.00	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=U415394&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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