Propanamide, 3-phenyl-N-ethyl-N-hexadecyl-

Inchi: InChI=1S/C27H47NO/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-20-25-28(4-2)27(29)24-23-2
InchiKey: XMEGDWJWKRRBLC-UHFFFAOYSA-N
Formula: C27H47NO
SMILES: CCCCCCCCCCCCCCCCN(CC)C(=O)CCc1ccccc1
Mol. weight [g/mol]: 401.67

Physical Properties

Property code	Value	Unit	Source
gf	270.73	kJ/mol	Joback Method
hf	-409.13	kJ/mol	Joback Method
hfus	64.35	kJ/mol	Joback Method
hvap	86.76	kJ/mol	Joback Method
log10ws	-8.57		Crippen Method
logp	7.949		Crippen Method
mcvol	379.080	ml/mol	McGowan Method
pc	855.96	kPa	Joback Method
rinpol	1797.00		NIST Webbook
rinpol	1797.00		NIST Webbook
tb	910.15	K	Joback Method
tc	1114.30	K	Joback Method
tf	502.87	K	Joback Method
vc	1.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1268.39	J/mol×K	910.15	Joback Method
cpg	1289.25	J/mol×K	944.17	Joback Method
cpg	1308.86	J/mol×K	978.20	Joback Method
cpg	1327.31	J/mol×K	1012.22	Joback Method
cpg	1344.68	J/mol×K	1046.25	Joback Method
cpg	1361.06	J/mol×K	1080.27	Joback Method
cpg	1376.54	J/mol×K	1114.30	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=U415405&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