Propanamide, 3-phenyl-N-ethyl-N-dodecyl-

Inchi: InChI=1S/C23H39NO/c1-3-5-6-7-8-9-10-11-12-16-21-24(4-2)23(25)20-19-22-17-14-13-15
InchiKey: RYAMYFMNZGUIRE-UHFFFAOYSA-N
Formula: C23H39NO
SMILES: CCCCCCCCCCCCN(CC)C(=O)CCc1ccccc1
Mol. weight [g/mol]: 345.56

Physical Properties

Property code	Value	Unit	Source
gf	237.05	kJ/mol	Joback Method
hf	-326.57	kJ/mol	Joback Method
hfus	53.99	kJ/mol	Joback Method
hvap	77.86	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	6.389		Crippen Method
mcvol	322.720	ml/mol	McGowan Method
pc	1086.35	kPa	Joback Method
rinpol	3104.00		NIST Webbook
rinpol	3104.00		NIST Webbook
tb	818.63	K	Joback Method
tc	1010.05	K	Joback Method
tf	457.79	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.68	J/mol×K	818.63	Joback Method
cpg	1037.13	J/mol×K	850.53	Joback Method
cpg	1055.46	J/mol×K	882.44	Joback Method
cpg	1072.74	J/mol×K	914.34	Joback Method
cpg	1089.04	J/mol×K	946.24	Joback Method
cpg	1104.42	J/mol×K	978.15	Joback Method
cpg	1118.92	J/mol×K	1010.05	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=U415403&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