Propanamide, N,N-dihexyl-3-phenyl-

Inchi: InChI=1S/C21H35NO/c1-3-5-7-12-18-22(19-13-8-6-4-2)21(23)17-16-20-14-10-9-11-15-2
InchiKey: DWWGRGZSSZIIPB-UHFFFAOYSA-N
Formula: C21H35NO
SMILES: CCCCCCN(CCCCCC)C(=O)CCc1ccccc1
Mol. weight [g/mol]: 317.51

Physical Properties

Property code	Value	Unit	Source
gf	220.21	kJ/mol	Joback Method
hf	-285.29	kJ/mol	Joback Method
hfus	48.81	kJ/mol	Joback Method
hvap	73.41	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.608		Crippen Method
mcvol	294.540	ml/mol	McGowan Method
pc	1238.09	kPa	Joback Method
rinpol	2369.00		NIST Webbook
tb	772.87	K	Joback Method
tc	962.42	K	Joback Method
tf	435.25	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.71	J/mol×K	772.87	Joback Method
cpg	915.67	J/mol×K	804.46	Joback Method
cpg	933.55	J/mol×K	836.05	Joback Method
cpg	950.42	J/mol×K	867.65	Joback Method
cpg	966.33	J/mol×K	899.24	Joback Method
cpg	981.32	J/mol×K	930.83	Joback Method
cpg	995.47	J/mol×K	962.42	Joback Method

Sources

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=U308214&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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