Propanamide, N,N-diundecyl-3-phenyl-

Inchi: InChI=1S/C31H55NO/c1-3-5-7-9-11-13-15-17-22-28-32(29-23-18-16-14-12-10-8-6-4-2)3
InchiKey: HGOHNEYPGWPFEF-UHFFFAOYSA-N
Formula: C31H55NO
SMILES: CCCCCCCCCCCN(CCCCCCCCCCC)C(=O)CCc1ccccc1
Mol. weight [g/mol]: 457.77

Physical Properties

Property code	Value	Unit	Source
gf	304.41	kJ/mol	Joback Method
hf	-491.69	kJ/mol	Joback Method
hfus	74.71	kJ/mol	Joback Method
hvap	95.66	kJ/mol	Joback Method
log10ws	-10.25		Crippen Method
logp	9.509		Crippen Method
mcvol	435.440	ml/mol	McGowan Method
pc	691.79	kPa	Joback Method
tb	1001.67	K	Joback Method
tc	1234.09	K	Joback Method
tf	547.95	K	Joback Method
vc	1.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1528.21	J/mol×K	1001.67	Joback Method
cpg	1551.56	J/mol×K	1040.41	Joback Method
cpg	1573.39	J/mol×K	1079.14	Joback Method
cpg	1593.85	J/mol×K	1117.88	Joback Method
cpg	1613.09	J/mol×K	1156.62	Joback Method
cpg	1631.26	J/mol×K	1195.36	Joback Method
cpg	1648.48	J/mol×K	1234.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308222&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume