Propanamide, 3-phenyl-N-ethyl-N-nonyl-

Inchi: InChI=1S/C20H33NO/c1-3-5-6-7-8-9-13-18-21(4-2)20(22)17-16-19-14-11-10-12-15-19/h1
InchiKey: IKFICLVYKVBYAH-UHFFFAOYSA-N
Formula: C20H33NO
SMILES: CCCCCCCCCN(CC)C(=O)CCc1ccccc1
Mol. weight [g/mol]: 303.48

Physical Properties

Property code	Value	Unit	Source
gf	211.79	kJ/mol	Joback Method
hf	-264.65	kJ/mol	Joback Method
hfus	46.22	kJ/mol	Joback Method
hvap	71.18	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	5.218		Crippen Method
mcvol	280.450	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
rinpol	2584.00		NIST Webbook
rinpol	2584.00		NIST Webbook
tb	749.99	K	Joback Method
tc	939.54	K	Joback Method
tf	423.98	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.52	J/mol×K	749.99	Joback Method
cpg	856.26	J/mol×K	781.58	Joback Method
cpg	873.93	J/mol×K	813.17	Joback Method
cpg	890.61	J/mol×K	844.76	Joback Method
cpg	906.32	J/mol×K	876.35	Joback Method
cpg	921.14	J/mol×K	907.94	Joback Method
cpg	935.11	J/mol×K	939.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415400&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume