Propanamide, 3-phenyl-N-ethyl-N-octyl-

Inchi: InChI=1S/C19H31NO/c1-3-5-6-7-8-12-17-20(4-2)19(21)16-15-18-13-10-9-11-14-18/h9-1
InchiKey: SXHMLFFFKQLOOA-UHFFFAOYSA-N
Formula: C19H31NO
SMILES: CCCCCCCCN(CC)C(=O)CCc1ccccc1
Mol. weight [g/mol]: 289.46

Physical Properties

Property code	Value	Unit	Source
gf	203.37	kJ/mol	Joback Method
hf	-244.01	kJ/mol	Joback Method
hfus	43.63	kJ/mol	Joback Method
hvap	68.95	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.828		Crippen Method
mcvol	266.360	ml/mol	McGowan Method
pc	1423.99	kPa	Joback Method
rinpol	2479.00		NIST Webbook
rinpol	2479.00		NIST Webbook
tb	727.11	K	Joback Method
tc	917.20	K	Joback Method
tf	412.71	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.27	J/mol×K	727.11	Joback Method
cpg	797.79	J/mol×K	758.79	Joback Method
cpg	815.27	J/mol×K	790.47	Joback Method
cpg	831.74	J/mol×K	822.15	Joback Method
cpg	847.26	J/mol×K	853.84	Joback Method
cpg	861.89	J/mol×K	885.52	Joback Method
cpg	875.67	J/mol×K	917.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415399&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

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