Propanamide, N-heptyl-N-octyl-3-phenyl-

Inchi: InChI=1S/C24H41NO/c1-3-5-7-9-11-16-22-25(21-15-10-8-6-4-2)24(26)20-19-23-17-13-1
InchiKey: IBCXEYMZEQZVRQ-UHFFFAOYSA-N
Formula: C24H41NO
SMILES: CCCCCCCCN(CCCCCCC)C(=O)CCc1ccccc1
Mol. weight [g/mol]: 359.59

Physical Properties

Property code	Value	Unit	Source
gf	245.47	kJ/mol	Joback Method
hf	-347.21	kJ/mol	Joback Method
hfus	56.58	kJ/mol	Joback Method
hvap	80.08	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	6.779		Crippen Method
mcvol	336.810	ml/mol	McGowan Method
pc	1020.73	kPa	Joback Method
rinpol	2664.00		NIST Webbook
rinpol	2664.00		NIST Webbook
tb	841.51	K	Joback Method
tc	1034.90	K	Joback Method
tf	469.06	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1079.35	J/mol×K	841.51	Joback Method
cpg	1099.07	J/mol×K	873.74	Joback Method
cpg	1117.67	J/mol×K	905.97	Joback Method
cpg	1135.19	J/mol×K	938.20	Joback Method
cpg	1151.71	J/mol×K	970.43	Joback Method
cpg	1167.29	J/mol×K	1002.67	Joback Method
cpg	1182.00	J/mol×K	1034.90	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=U308218&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

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