Propanamide, N,N-didecyl-3-phenyl-

Inchi: InChI=1S/C29H51NO/c1-3-5-7-9-11-13-15-20-26-30(27-21-16-14-12-10-8-6-4-2)29(31)25
InchiKey: XVDHBPPZWJVSNZ-UHFFFAOYSA-N
Formula: C29H51NO
SMILES: CCCCCCCCCCN(CCCCCCCCCC)C(=O)CCc1ccccc1
Mol. weight [g/mol]: 429.72

Physical Properties

Property code	Value	Unit	Source
gf	287.57	kJ/mol	Joback Method
hf	-450.41	kJ/mol	Joback Method
hfus	69.53	kJ/mol	Joback Method
hvap	91.21	kJ/mol	Joback Method
log10ws	-9.41		Crippen Method
logp	8.729		Crippen Method
mcvol	407.260	ml/mol	McGowan Method
pc	767.34	kPa	Joback Method
rinpol	3307.00		NIST Webbook
tb	955.91	K	Joback Method
tc	1171.95	K	Joback Method
tf	525.41	K	Joback Method
vc	1.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1397.32	J/mol×K	955.91	Joback Method
cpg	1419.26	J/mol×K	991.92	Joback Method
cpg	1439.83	J/mol×K	1027.92	Joback Method
cpg	1459.15	J/mol×K	1063.93	Joback Method
cpg	1477.32	J/mol×K	1099.94	Joback Method
cpg	1494.46	J/mol×K	1135.94	Joback Method
cpg	1510.67	J/mol×K	1171.95	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U308221&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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