Propanamide, N,N-diundecyl-2,2-dimethyl-

Inchi: InChI=1S/C27H55NO/c1-6-8-10-12-14-16-18-20-22-24-28(26(29)27(3,4)5)25-23-21-19-1
InchiKey: ZCJRDYFSTZWJHW-UHFFFAOYSA-N
Formula: C27H55NO
SMILES: CCCCCCCCCCCN(CCCCCCCCCCC)C(=O)C(C)(C)C
Mol. weight [g/mol]: 409.73

Physical Properties

Property code	Value	Unit	Source
gf	161.16	kJ/mol	Joback Method
hf	-654.41	kJ/mol	Joback Method
hfus	62.89	kJ/mol	Joback Method
hvap	83.19	kJ/mol	Joback Method
log10ws	-9.23		Crippen Method
logp	8.923		Crippen Method
mcvol	402.840	ml/mol	McGowan Method
pc	718.76	kPa	Joback Method
rinpol	2807.00		NIST Webbook
tb	880.24	K	Joback Method
tc	1078.67	K	Joback Method
tf	478.87	K	Joback Method
vc	1.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1361.33	J/mol×K	880.24	Joback Method
cpg	1384.89	J/mol×K	913.31	Joback Method
cpg	1407.17	J/mol×K	946.38	Joback Method
cpg	1428.26	J/mol×K	979.45	Joback Method
cpg	1448.24	J/mol×K	1012.52	Joback Method
cpg	1467.21	J/mol×K	1045.60	Joback Method
cpg	1485.25	J/mol×K	1078.67	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=U308133&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