Propanamide, N,N-diundecyl-2-methyl-

Inchi: InChI=1S/C26H53NO/c1-5-7-9-11-13-15-17-19-21-23-27(26(28)25(3)4)24-22-20-18-16-1
InchiKey: WYUVZLVAZKNPBE-UHFFFAOYSA-N
Formula: C26H53NO
SMILES: CCCCCCCCCCCN(CCCCCCCCCCC)C(=O)C(C)C
Mol. weight [g/mol]: 395.71

Physical Properties

Property code	Value	Unit	Source
gf	147.46	kJ/mol	Joback Method
hf	-630.30	kJ/mol	Joback Method
hfus	64.19	kJ/mol	Joback Method
hvap	81.87	kJ/mol	Joback Method
log10ws	-8.81		Crippen Method
logp	8.533		Crippen Method
mcvol	388.750	ml/mol	McGowan Method
pc	752.67	kPa	Joback Method
rinpol	2751.00		NIST Webbook
tb	860.15	K	Joback Method
tc	1053.76	K	Joback Method
tf	450.18	K	Joback Method
vc	1.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1296.53	J/mol×K	860.15	Joback Method
cpg	1319.75	J/mol×K	892.42	Joback Method
cpg	1341.68	J/mol×K	924.69	Joback Method
cpg	1362.41	J/mol×K	956.95	Joback Method
cpg	1381.99	J/mol×K	989.22	Joback Method
cpg	1400.48	J/mol×K	1021.49	Joback Method
cpg	1417.96	J/mol×K	1053.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308090&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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