Propanamide, N,N-diundecyl-2-chloro-

Inchi: InChI=1S/C25H50ClNO/c1-4-6-8-10-12-14-16-18-20-22-27(25(28)24(3)26)23-21-19-17-1
InchiKey: USMDOBCIJVLEJB-UHFFFAOYSA-N
Formula: C25H50ClNO
SMILES: CCCCCCCCCCCN(CCCCCCCCCCC)C(=O)C(C)Cl
Mol. weight [g/mol]: 416.12

Physical Properties

Property code	Value	Unit	Source
gf	127.11	kJ/mol	Joback Method
hf	-625.40	kJ/mol	Joback Method
hfus	65.80	kJ/mol	Joback Method
hvap	84.03	kJ/mol	Joback Method
log10ws	-8.90		Crippen Method
logp	8.504		Crippen Method
mcvol	386.900	ml/mol	McGowan Method
pc	777.64	kPa	Joback Method
rinpol	2877.00		NIST Webbook
rinpol	2877.00		NIST Webbook
tb	874.70	K	Joback Method
tc	1071.38	K	Joback Method
tf	468.83	K	Joback Method
vc	1.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1267.86	J/mol×K	874.70	Joback Method
cpg	1289.72	J/mol×K	907.48	Joback Method
cpg	1310.33	J/mol×K	940.26	Joback Method
cpg	1329.79	J/mol×K	973.04	Joback Method
cpg	1348.14	J/mol×K	1005.82	Joback Method
cpg	1365.47	J/mol×K	1038.60	Joback Method
cpg	1381.84	J/mol×K	1071.38	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=U308393&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