

Propanamide, N-decyl-N-methyl-2-chloro-

Inchi:	InChI=1S/C14H28ClNO/c1-4-5-6-7-8-9-10-11-12-16(3)14(17)13(2)15/h13H,4-12H2,1-3H
InchiKey:	LJUWACZMRIHSY-UHFFFAOYSA-N
Formula:	C14H28ClNO
SMILES:	CCCCCCCCCN(C)C(=O)C(C)Cl
Mol. weight [g/mol]:	261.83

Physical Properties

Property code	Value	Unit	Source
gf	34.49	kJ/mol	Joback Method
hf	-398.36	kJ/mol	Joback Method
hfus	37.31	kJ/mol	Joback Method
hvap	59.54	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	4.213		Crippen Method
mvol	231.910	ml/mol	McGowan Method
pc	1562.28	kPa	Joback Method
rinpol	1879.00		NIST Webbook
tb	623.02	K	Joback Method
tc	797.36	K	Joback Method
tf	344.86	K	Joback Method
vc	0.886	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.23	J/mol×K	623.02	Joback Method
cpg	628.26	J/mol×K	652.08	Joback Method
cpg	644.49	J/mol×K	681.13	Joback Method
cpg	659.94	J/mol×K	710.19	Joback Method
cpg	674.64	J/mol×K	739.25	Joback Method
cpg	688.61	J/mol×K	768.31	Joback Method
cpg	701.88	J/mol×K	797.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308386&Units=SI

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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