Propanamide, N,N-dioctyl-2-chloro-

Inchi: InChI=1S/C19H38ClNO/c1-4-6-8-10-12-14-16-21(19(22)18(3)20)17-15-13-11-9-7-5-2/h1
InchiKey: SFIDWMGWNSNDKS-UHFFFAOYSA-N
Formula: C19H38ClNO
SMILES: CCCCCCCCN(CCCCCCCC)C(=O)C(C)Cl
Mol. weight [g/mol]: 331.96

Physical Properties

Property code	Value	Unit	Source
gf	76.59	kJ/mol	Joback Method
hf	-501.56	kJ/mol	Joback Method
hfus	50.26	kJ/mol	Joback Method
hvap	70.67	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	6.163		Crippen Method
mcvol	302.360	ml/mol	McGowan Method
pc	1103.74	kPa	Joback Method
rinpol	2266.00		NIST Webbook
rinpol	2266.00		NIST Webbook
tb	737.42	K	Joback Method
tc	912.64	K	Joback Method
tf	401.21	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	895.41	J/mol×K	737.42	Joback Method
cpg	914.37	J/mol×K	766.62	Joback Method
cpg	932.39	J/mol×K	795.83	Joback Method
cpg	949.51	J/mol×K	825.03	Joback Method
cpg	965.78	J/mol×K	854.23	Joback Method
cpg	981.22	J/mol×K	883.44	Joback Method
cpg	995.88	J/mol×K	912.64	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=U308390&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