Propanamide, N,N-dioctyl-3-chloro-

Inchi: InChI=1S/C19H38ClNO/c1-3-5-7-9-11-13-17-21(19(22)15-16-20)18-14-12-10-8-6-4-2/h3-
InchiKey: SLCJNBBZBLGJLW-UHFFFAOYSA-N
Formula: C19H38ClNO
SMILES: CCCCCCCCN(CCCCCCCC)C(=O)CCCl
Mol. weight [g/mol]: 331.96

Physical Properties

Property code	Value	Unit	Source
gf	79.03	kJ/mol	Joback Method
hf	-496.28	kJ/mol	Joback Method
hfus	53.78	kJ/mol	Joback Method
hvap	71.06	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	6.165		Crippen Method
mcvol	302.360	ml/mol	McGowan Method
pc	1097.90	kPa	Joback Method
rinpol	2361.00		NIST Webbook
rinpol	2361.00		NIST Webbook
tb	737.86	K	Joback Method
tc	911.70	K	Joback Method
tf	416.21	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	894.96	J/mol×K	737.86	Joback Method
cpg	913.75	J/mol×K	766.83	Joback Method
cpg	931.63	J/mol×K	795.81	Joback Method
cpg	948.63	J/mol×K	824.78	Joback Method
cpg	964.79	J/mol×K	853.75	Joback Method
cpg	980.15	J/mol×K	882.73	Joback Method
cpg	994.74	J/mol×K	911.70	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=U308507&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
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