Propanamide, N,N-dibutyl-2-chloro-

Inchi: InChI=1S/C11H22ClNO/c1-4-6-8-13(9-7-5-2)11(14)10(3)12/h10H,4-9H2,1-3H3
InchiKey: AMBSMXGFOZRXNX-UHFFFAOYSA-N
Formula: C11H22ClNO
SMILES: CCCCN(CCCC)C(=O)C(C)Cl
Mol. weight [g/mol]: 219.75

Physical Properties

Property code	Value	Unit	Source
gf	9.23	kJ/mol	Joback Method
hf	-336.44	kJ/mol	Joback Method
hfus	29.54	kJ/mol	Joback Method
hvap	52.87	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	3.043		Crippen Method
mcvol	189.640	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	1494.00		NIST Webbook
tb	554.38	K	Joback Method
tc	732.55	K	Joback Method
tf	311.05	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.41	J/mol×K	554.38	Joback Method
cpg	471.90	J/mol×K	584.07	Joback Method
cpg	486.66	J/mol×K	613.77	Joback Method
cpg	500.70	J/mol×K	643.46	Joback Method
cpg	514.06	J/mol×K	673.16	Joback Method
cpg	526.75	J/mol×K	702.85	Joback Method
cpg	538.81	J/mol×K	732.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308383&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

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