1-Propanamine, 3-chloro-N,N-diethyl-

Other names: 3-chloropropyl(diethyl)amine
Inchi: InChI=1S/C7H16ClN/c1-3-9(4-2)7-5-6-8/h3-7H2,1-2H3
InchiKey: WVUULNDRFBHTFG-UHFFFAOYSA-N
Formula: C7H16ClN
SMILES: CCN(CC)CCCCl
Mol. weight [g/mol]: 149.66
CAS: 104-77-8

Physical Properties

Property code	Value	Unit	Source
gf	106.91	kJ/mol	Joback Method
hf	-136.02	kJ/mol	Joback Method
hfus	21.10	kJ/mol	Joback Method
hvap	37.60	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.957		Crippen Method
mcvol	131.710	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	975.00		NIST Webbook
tb	409.43	K	Joback Method
tc	579.67	K	Joback Method
tf	231.04	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.07	J/mol×K	409.43	Joback Method
cpg	264.79	J/mol×K	437.80	Joback Method
cpg	276.97	J/mol×K	466.18	Joback Method
cpg	288.63	J/mol×K	494.55	Joback Method
cpg	299.78	J/mol×K	522.92	Joback Method
cpg	310.44	J/mol×K	551.30	Joback Method
cpg	320.63	J/mol×K	579.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104778&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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