1-Diethylamino-2-chloropropane

Other names: 2-chloropropyl(diethyl)amine
Inchi: InChI=1S/C7H16ClN/c1-4-9(5-2)6-7(3)8/h7H,4-6H2,1-3H3
InchiKey: QOHJWGXVMZSTAZ-UHFFFAOYSA-N
Formula: C7H16ClN
SMILES: CCN(CC)CC(C)Cl
Mol. weight [g/mol]: 149.66
CAS: 761-21-7

Physical Properties

Property code	Value	Unit	Source
gf	104.47	kJ/mol	Joback Method
hf	-141.30	kJ/mol	Joback Method
hfus	17.58	kJ/mol	Joback Method
hvap	37.22	kJ/mol	Joback Method
log10ws	-1.59		Crippen Method
logp	1.955		Crippen Method
mcvol	131.710	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	924.00		NIST Webbook
tb	408.99	K	Joback Method
tc	583.10	K	Joback Method
tf	216.04	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.04	J/mol×K	408.99	Joback Method
cpg	265.14	J/mol×K	438.01	Joback Method
cpg	277.66	J/mol×K	467.03	Joback Method
cpg	289.63	J/mol×K	496.04	Joback Method
cpg	301.07	J/mol×K	525.06	Joback Method
cpg	311.99	J/mol×K	554.08	Joback Method
cpg	322.41	J/mol×K	583.10	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=C761217&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