Aniline, N,N-di(3-chloropropyl)-

Inchi: InChI=1S/C12H17Cl2N/c13-8-4-10-15(11-5-9-14)12-6-2-1-3-7-12/h1-3,6-7H,4-5,8-11H2
InchiKey: DPGPWVSHZFFFDN-UHFFFAOYSA-N
Formula: C12H17Cl2N
SMILES: ClCCCN(CCCCl)c1ccccc1
Mol. weight [g/mol]: 246.18

Physical Properties

Property code	Value	Unit	Source
gf	249.49	kJ/mol	Joback Method
hf	-18.43	kJ/mol	Joback Method
hfus	32.29	kJ/mol	Joback Method
hvap	55.39	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.751		Crippen Method
mcvol	190.640	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rinpol	1913.00		NIST Webbook
rinpol	1913.00		NIST Webbook
tb	587.94	K	Joback Method
tc	793.78	K	Joback Method
tf	343.73	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.05	J/mol×K	587.94	Joback Method
cpg	457.53	J/mol×K	622.25	Joback Method
cpg	472.03	J/mol×K	656.55	Joback Method
cpg	485.60	J/mol×K	690.86	Joback Method
cpg	498.30	J/mol×K	725.17	Joback Method
cpg	510.16	J/mol×K	759.47	Joback Method
cpg	521.25	J/mol×K	793.78	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=U380844&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