Aniline, 2-chloro-n-isopropyl-

Inchi: InChI=1S/C9H12ClN/c1-7(2)11-9-6-4-3-5-8(9)10/h3-7,11H,1-2H3
InchiKey: JCRMYLUIMGTZSR-UHFFFAOYSA-N
Formula: C9H12ClN
SMILES: CC(C)Nc1ccccc1Cl
Mol. weight [g/mol]: 169.65
CAS: 78235-07-1

Physical Properties

Property code	Value	Unit	Source
gf	202.70	kJ/mol	Joback Method
hf	28.42	kJ/mol	Joback Method
hfus	18.49	kJ/mol	Joback Method
hvap	49.00	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	3.160		Crippen Method
mcvol	136.130	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
tb	524.14	K	Joback Method
tc	744.97	K	Joback Method
tf	297.71	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.98	J/mol×K	524.14	Joback Method
cpg	301.47	J/mol×K	560.94	Joback Method
cpg	314.13	J/mol×K	597.75	Joback Method
cpg	325.98	J/mol×K	634.55	Joback Method
cpg	337.07	J/mol×K	671.36	Joback Method
cpg	347.43	J/mol×K	708.16	Joback Method
cpg	357.10	J/mol×K	744.97	Joback Method

Sources

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=C78235071&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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