

N-n-butyl-2-chloroaniline

Inchi:	InChI=1S/C10H14ClN/c1-2-3-8-12-10-7-5-4-6-9(10)11/h4-7,12H,2-3,8H2,1H3
InchiKey:	LJRWSALKDLMPRE-UHFFFAOYSA-N
Formula:	C10H14ClN
SMILES:	CCCCNc1ccccc1Cl
Mol. weight [g/mol]:	183.68
CAS:	939-61-7

Physical Properties

Property code	Value	Unit	Source
gf	213.56	kJ/mol	Joback Method
hf	13.06	kJ/mol	Joback Method
hfus	24.60	kJ/mol	Joback Method
hvap	51.61	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.552		Crippen Method
mvol	150.220	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
tb	547.46	K	Joback Method
tc	759.81	K	Joback Method
tf	323.98	K	Joback Method
vc	0.572	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.86	J/mol×K	547.46	Joback Method
cpg	346.86	J/mol×K	582.85	Joback Method
cpg	360.03	J/mol×K	618.24	Joback Method
cpg	372.41	J/mol×K	653.64	Joback Method
cpg	384.04	J/mol×K	689.03	Joback Method
cpg	394.93	J/mol×K	724.42	Joback Method
cpg	405.14	J/mol×K	759.81	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=C939617&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
mccvol:	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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