1-(4-Chloroanilino)-2-propanol

Inchi: InChI=1S/C9H12ClNO/c1-7(12)6-11-9-4-2-8(10)3-5-9/h2-5,7,11-12H,6H2,1H3
InchiKey: ZJQJJRAOBNZRIF-UHFFFAOYSA-N
Formula: C9H12ClNO
SMILES: CC(O)CNc1ccc(Cl)cc1
Mol. weight [g/mol]: 185.65
CAS: 72506-83-3

Physical Properties

Property code	Value	Unit	Source
gf	65.88	kJ/mol	Joback Method
hf	-123.81	kJ/mol	Joback Method
hfus	22.58	kJ/mol	Joback Method
hvap	65.68	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.133		Crippen Method
mcvol	142.000	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
tb	616.32	K	Joback Method
tc	821.27	K	Joback Method
tf	358.53	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.19	J/mol×K	616.32	Joback Method
cpg	348.10	J/mol×K	650.48	Joback Method
cpg	358.34	J/mol×K	684.64	Joback Method
cpg	367.94	J/mol×K	718.79	Joback Method
cpg	376.93	J/mol×K	752.95	Joback Method
cpg	385.34	J/mol×K	787.11	Joback Method
cpg	393.19	J/mol×K	821.27	Joback Method

Sources

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=C72506833&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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