

Aniline, 2-tert-butyl-4,5-dichloro-

Inchi:	InChI=1S/C10H13Cl2N/c1-10(2,3)6-4-7(11)8(12)5-9(6)13/h4-5H,13H2,1-3H3
InchiKey:	RQDBUUPMQBPUGF-UHFFFAOYSA-N
Formula:	C10H13Cl2N
SMILES:	CC(C)(C)c1cc(Cl)c(Cl)cc1N
Mol. weight [g/mol]:	218.12

Physical Properties

Property code	Value	Unit	Source
gf	162.27	kJ/mol	Joback Method
hf	-54.05	kJ/mol	Joback Method
hfus	20.71	kJ/mol	Joback Method
hvap	60.23	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.873		Crippen Method
mcvol	162.460	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
tb	613.98	K	Joback Method
tc	855.32	K	Joback Method
tf	411.96	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.16	J/mol×K	613.98	Joback Method
cpg	383.09	J/mol×K	654.20	Joback Method
cpg	395.07	J/mol×K	694.43	Joback Method
cpg	406.16	J/mol×K	734.65	Joback Method
cpg	416.42	J/mol×K	774.88	Joback Method
cpg	425.93	J/mol×K	815.10	Joback Method
cpg	434.73	J/mol×K	855.32	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=B6009256&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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