

Aniline, 2-tert-butyl-n-(o-chlorobenzyl)-

Inchi:	InChI=1S/C17H20ClN/c1-17(2,3)14-9-5-7-11-16(14)19-12-13-8-4-6-10-15(13)18/h4-11,1
InchiKey:	DAIQAPHLUWCHQE-UHFFFAOYSA-N
Formula:	C17H20ClN
SMILES:	CC(C)(C)c1ccccc1NCc1ccccc1Cl
Mol. weight [g/mol]:	273.80

Physical Properties

Property code	Value	Unit	Source
gf	378.12	kJ/mol	Joback Method
hf	84.89	kJ/mol	Joback Method
hfus	28.97	kJ/mol	Joback Method
hvap	68.84	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	5.250		Crippen Method
mcvol	225.090	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
tb	736.05	K	Joback Method
tc	976.97	K	Joback Method
tf	444.23	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.31	J/molxK	736.05	Joback Method
cpg	627.15	J/molxK	776.20	Joback Method
cpg	642.66	J/molxK	816.36	Joback Method
cpg	656.97	J/molxK	856.51	Joback Method
cpg	670.17	J/molxK	896.66	Joback Method
cpg	682.39	J/molxK	936.81	Joback Method
cpg	693.72	J/molxK	976.97	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=B6009258&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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