

Aniline, 2-tert-butyl-n-cyclohexyl-

Inchi:	InChI=1S/C16H25N/c1-16(2,3)14-11-7-8-12-15(14)17-13-9-5-4-6-10-13/h7-8,11-13,17H,
InchiKey:	OLRNQABQSVROHA-UHFFFAOYSA-N
Formula:	C16H25N
SMILES:	CC(C)(C)c1ccccc1NC1CCCCC1
Mol. weight [g/mol]:	231.38
CAS:	202276-37-7

Physical Properties

Property code	Value	Unit	Source
gf	303.30	kJ/mol	Joback Method
hf	-49.47	kJ/mol	Joback Method
hfus	20.37	kJ/mol	Joback Method
hvap	59.72	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.729		Crippen Method
mcvol	211.660	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
tb	663.63	K	Joback Method
tc	899.01	K	Joback Method
tf	371.48	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.60	J/molxK	663.63	Joback Method
cpg	623.99	J/molxK	702.86	Joback Method
cpg	644.71	J/molxK	742.09	Joback Method
cpg	663.87	J/molxK	781.32	Joback Method
cpg	681.57	J/molxK	820.55	Joback Method
cpg	697.91	J/molxK	859.78	Joback Method
cpg	712.98	J/molxK	899.01	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C202276377&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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