

trans,trans-2,5-Di-tert-butylcyclohexanol

Inchi:	InChI=1S/C14H28O/c1-13(2,3)10-7-8-11(12(15)9-10)14(4,5)6/h10-12,15H,7-9H2,1-6H3/
InchiKey:	REPJSEOIEYLARO-SRVKXCTJSA-N
Formula:	C14H28O
SMILES:	CC(C)(C)C1CCC(C(C)(C)C)C(O)C1
Mol. weight [g/mol]:	212.37
CAS:	24418-07-3

Physical Properties

Property code	Value	Unit	Source
gf	-55.11	kJ/mol	Joback Method
hf	-488.38	kJ/mol	Joback Method
hfus	15.25	kJ/mol	Joback Method
hvap	60.66	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.856		Crippen Method
mcvol	203.130	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
tb	615.65	K	Joback Method
tc	812.88	K	Joback Method
tf	312.10	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.46	J/molxK	615.65	Joback Method
cpg	604.34	J/molxK	648.52	Joback Method
cpg	623.98	J/molxK	681.39	Joback Method
cpg	642.44	J/molxK	714.27	Joback Method
cpg	659.78	J/molxK	747.14	Joback Method
cpg	676.05	J/molxK	780.01	Joback Method
cpg	691.30	J/molxK	812.88	Joback Method
dvisc	0.0155906	Paxs	312.10	Joback Method
dvisc	0.0033236	Paxs	362.69	Joback Method

dvisc	0.0010344	Paxs	413.28	Joback Method
dvisc	0.0004153	Paxs	463.88	Joback Method
dvisc	0.0001995	Paxs	514.47	Joback Method
dvisc	0.0001093	Paxs	565.06	Joback Method
dvisc	0.0000661	Paxs	615.65	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=C24418073&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
dvisc:	Dynamic viscosity
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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