4-t-Butylcyclohexanone diethylacetal

Other names: 4-tert-Butylcyclohexanone diethyl acetal
Inchi: InChI=1S/C14H28O2/c1-6-15-14(16-7-2)10-8-12(9-11-14)13(3,4)5/h12H,6-11H2,1-5H3
InchiKey: QTSXNUWFLGKEKB-UHFFFAOYSA-N
Formula: C14H28O2
SMILES: CCOC1(OCC)CCC(C(C)(C)C)CC1
Mol. weight [g/mol]: 228.38

Physical Properties

Property code	Value	Unit	Source
hfus	13.59	kJ/mol	Joback Method
ie	8.90	eV	Cheméo Relay (1.0)
logp	3.992		Crippen Method
mcvol	209.000	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.08	J/mol×K	576.45	Joback Method
cpg	583.45	J/mol×K	610.24	Joback Method
cpg	604.63	J/mol×K	644.03	Joback Method
cpg	624.72	J/mol×K	677.82	Joback Method
cpg	643.81	J/mol×K	711.61	Joback Method
cpg	661.99	J/mol×K	745.41	Joback Method
cpg	679.35	J/mol×K	779.20	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	402.50 ± 0.50	K	2.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1900589&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure