

1,3-Dioxolane, 2,4-di-tert-butyl-, trans-

Inchi:	InChI=1S/C11H22O2/c1-10(2,3)8-7-12-9(13-8)11(4,5)6/h8-9H,7H2,1-6H3/t8-,9+/m1/s1
InchiKey:	WENPMVZGWLEFAM-BDAKNGLRSA-N
Formula:	C11H22O2
SMILES:	CC(C)(C)C1COC(C(C)(C)C)O1
Mol. weight [g/mol]:	186.29
CAS:	26563-87-1

Physical Properties

Property code	Value	Unit	Source
gf	-95.98	kJ/mol	Joback Method
hf	-511.73	kJ/mol	Joback Method
hfus	20.38	kJ/mol	Joback Method
hvap	46.46	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.820		Crippen Method
mcvol	166.730	ml/mol	McGowan Method
pc	2252.53	kPa	Joback Method
tb	509.13	K	Joback Method
tc	719.54	K	Joback Method
tf	278.37	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.18	J/mol×K	509.13	Joback Method
cpg	442.23	J/mol×K	544.20	Joback Method
cpg	461.95	J/mol×K	579.27	Joback Method
cpg	480.40	J/mol×K	614.34	Joback Method
cpg	497.65	J/mol×K	649.40	Joback Method
cpg	513.77	J/mol×K	684.47	Joback Method
cpg	528.81	J/mol×K	719.54	Joback Method
dvisc	0.0075039	Pa×s	278.37	Joback Method
dvisc	0.0032143	Pa×s	316.83	Joback Method

dvisc	0.0016542	Pa×s	355.29	Joback Method
dvisc	0.0009693	Pa×s	393.75	Joback Method
dvisc	0.0006246	Pa×s	432.21	Joback Method
dvisc	0.0004325	Pa×s	470.67	Joback Method
dvisc	0.0003166	Pa×s	509.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26563871&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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