tolyaldehyde propylene glycol acetal

Other names: 4-methyl-2-(o-tolyl)-1,3-dioxolane
Inchi: InChI=1S/C11H14O2/c1-8-3-5-10(6-4-8)11-12-7-9(2)13-11/h3-6,9,11H,7H2,1-2H3
InchiKey: VPBUQMKUEPQXKR-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: Cc1ccc(C2OCC(C)O2)cc1
Mol. weight [g/mol]: 178.23
CAS: 58244-29-4

Physical Properties

Property code	Value	Unit	Source
gf	1.12	kJ/mol	Joback Method
hf	-269.17	kJ/mol	Joback Method
hfus	28.86	kJ/mol	Joback Method
hvap	51.99	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.429		Crippen Method
mcvol	142.970	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	1376.00		NIST Webbook
tb	547.25	K	Joback Method
tc	779.61	K	Joback Method
tf	312.47	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.04	J/mol×K	547.25	Joback Method
cpg	427.86	J/mol×K	740.88	Joback Method
cpg	414.43	J/mol×K	702.16	Joback Method
cpg	399.97	J/mol×K	663.43	Joback Method
cpg	384.44	J/mol×K	624.70	Joback Method
cpg	367.81	J/mol×K	585.98	Joback Method
cpg	440.30	J/mol×K	779.61	Joback Method

dvisc	0.0003348	Pa×s	547.25	Joback Method
dvisc	0.0004104	Pa×s	508.12	Joback Method
dvisc	0.0005203	Pa×s	468.99	Joback Method
dvisc	0.0006887	Pa×s	429.86	Joback Method
dvisc	0.0009645	Pa×s	390.73	Joback Method
dvisc	0.0014557	Pa×s	351.60	Joback Method
dvisc	0.0024358	Pa×s	312.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58244294&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume