1,3-Dioxolane, 2,4,5-trimethyl-

Other names: 2,4,5-Trimethyl-1,3-dioxolane
Inchi: InChI=1S/C6H12O2/c1-4-5(2)8-6(3)7-4/h4-6H,1-3H3
InchiKey: HLEXJAVJCZLRTH-UHFFFAOYSA-N
Formula: C6H12O2
SMILES: CC1OC(C)C(C)O1
Mol. weight [g/mol]: 116.16
CAS: 3299-32-9

Physical Properties

Property code	Value	Unit	Source
gf	-151.47	kJ/mol	Joback Method
hf	-411.37	kJ/mol	Joback Method
hfus	23.33	kJ/mol	Joback Method
hvap	37.61	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.156		Crippen Method
mcvol	96.280	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinpol	735.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	752.00		NIST Webbook
ripol	967.00		NIST Webbook
ripol	1020.00		NIST Webbook
ripol	967.00		NIST Webbook
ripol	1020.00		NIST Webbook
tb	396.52	K	Joback Method
tc	592.40	K	Joback Method
tf	212.94	K	Joback Method
vc	0.352	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.64	J/mol×K	396.52	Joback Method
cpg	209.33	J/mol×K	429.17	Joback Method
cpg	222.46	J/mol×K	461.81	Joback Method
cpg	235.05	J/mol×K	494.46	Joback Method
cpg	247.11	J/mol×K	527.10	Joback Method
cpg	258.62	J/mol×K	559.75	Joback Method
cpg	269.61	J/mol×K	592.40	Joback Method
dvisc	0.0019113	Pa×s	212.94	Joback Method
dvisc	0.0012317	Pa×s	243.54	Joback Method
dvisc	0.0008756	Pa×s	274.13	Joback Method
dvisc	0.0006666	Pa×s	304.73	Joback Method
dvisc	0.0005334	Pa×s	335.33	Joback Method
dvisc	0.0004430	Pa×s	365.92	Joback Method
dvisc	0.0003786	Pa×s	396.52	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=C3299329&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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