

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

Other names:	2,2,4-Trimethyl-1,3-dioxolane 2,2,4-Trimethyldioxolane
Inchi:	InChI=1S/C6H12O2/c1-5-4-7-6(2,3)8-5/h5H,4H2,1-3H3
InchiKey:	ALTFLAPROMVXNX-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CC1COC(C)(C)O1
Mol. weight [g/mol]:	116.16
CAS:	1193-11-9

Physical Properties

Property code	Value	Unit	Source
gf	-149.25	kJ/mol	Joback Method
hf	-375.79	kJ/mol	Joback Method
hfus	15.96	kJ/mol	Joback Method
hvap	36.77	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	1.158		Crippen Method
mcvol	96.280	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
tb	401.43	K	Joback Method
tc	606.93	K	Joback Method
tf	241.08	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.97	J/mol×K	401.43	Joback Method
cpg	210.15	J/mol×K	435.68	Joback Method
cpg	223.34	J/mol×K	469.93	Joback Method
cpg	235.64	J/mol×K	504.18	Joback Method
cpg	247.12	J/mol×K	538.43	Joback Method
cpg	257.87	J/mol×K	572.68	Joback Method
cpg	267.98	J/mol×K	606.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1193119&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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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