

1,3-Dioxolane, 2,2-dimethyl-4-(tert-butyloxymethyl)-

Inchi:	InChI=1S/C10H20O3/c1-9(2,3)11-6-8-7-12-10(4,5)13-8/h8H,6-7H2,1-5H3
InchiKey:	MHVCAGULIQFGCK-UHFFFAOYSA-N
Formula:	C10H20O3
SMILES:	CC(C)(C)OCC1COC(C)(C)O1
Mol. weight [g/mol]:	188.26

Physical Properties

Property code	Value	Unit	Source
gf	-217.73	kJ/mol	Joback Method
hf	-599.32	kJ/mol	Joback Method
hfus	20.10	kJ/mol	Joback Method
hvap	46.78	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.953		Crippen Method
mcvol	158.510	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1159.00		NIST Webbook
rinpol	1159.00		NIST Webbook
tb	512.14	K	Joback Method
tc	719.21	K	Joback Method
tf	310.81	K	Joback Method
vc	0.583	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.13	J/mol×K	512.14	Joback Method
cpg	416.50	J/mol×K	546.65	Joback Method
cpg	433.74	J/mol×K	581.16	Joback Method
cpg	449.95	J/mol×K	615.67	Joback Method
cpg	465.24	J/mol×K	650.19	Joback Method
cpg	479.71	J/mol×K	684.70	Joback Method
cpg	493.46	J/mol×K	719.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381762&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvpap:	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
rinpól:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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