

1,3-Dioxolane, 4-(chloromethyl)-2,2-dimethyl-

Other names:	4-(Chloromethyl)-2,2-dimethyl-1,3-dioxolane
Inchi:	InChI=1S/C6H11ClO2/c1-6(2)8-4-5(3-7)9-6/h5H,3-4H2,1-2H3
InchiKey:	BNPOTXLWPZOESZ-UHFFFAOYSA-N
Formula:	C6H11ClO2
SMILES:	CC1(C)OCC(CCl)O1
Mol. weight [g/mol]:	150.60
CAS:	4362-40-7

Physical Properties

Property code	Value	Unit	Source
gf	-161.18	kJ/mol	Joback Method
hf	-391.53	kJ/mol	Joback Method
hfus	20.16	kJ/mol	Joback Method
hvap	41.15	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	1.377		Crippen Method
mcvol	108.520	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
tb	438.86	K	Joback Method
tc	651.86	K	Joback Method
tf	271.00	K	Joback Method
vc	0.401	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.11	J/mol×K	438.86	Joback Method
cpg	237.46	J/mol×K	474.36	Joback Method
cpg	249.83	J/mol×K	509.86	Joback Method
cpg	261.33	J/mol×K	545.36	Joback Method
cpg	272.05	J/mol×K	580.86	Joback Method
cpg	282.09	J/mol×K	616.36	Joback Method
cpg	291.55	J/mol×K	651.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4362407&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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