1,3-Dioxolane, 2-(3-chloropropyl)-2-methyl-

Other names: 2,2-(Ethylenedioxy)-5-chloropentane
5-Chloro-2-pentanone ethylene ketal
2-(3-chloropropyl)-2-methyl-1,3-dioxolane
Inchi: InChI=1S/C7H13ClO2/c1-7(3-2-4-8)9-5-6-10-7/h2-6H2,1H3
InchiKey: OFERIRWCHSOJJT-UHFFFAOYSA-N
Formula: C7H13ClO2
SMILES: CC1(CCCCl)OCCO1
Mol. weight [g/mol]: 164.63
CAS: 5978-08-5

Physical Properties

Property code	Value	Unit	Source
gf	-145.05	kJ/mol	Joback Method
hf	-391.83	kJ/mol	Joback Method
hfus	21.68	kJ/mol	Joback Method
hvap	43.69	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.768		Crippen Method
mcvol	122.610	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
tb	466.41	K	Joback Method
tc	676.87	K	Joback Method
tf	286.51	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.55	J/mol×K	466.41	Joback Method
cpg	278.51	J/mol×K	501.49	Joback Method
cpg	291.48	J/mol×K	536.56	Joback Method
cpg	303.54	J/mol×K	571.64	Joback Method
cpg	314.82	J/mol×K	606.71	Joback Method
cpg	325.41	J/mol×K	641.79	Joback Method

cpg	335.41	J/mol×K	676.87	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	347.70	K	0.90	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5978085&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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