Gamma-chloromethyl-gamma-butyrolactone

Inchi: InChI=1S/C5H7ClO2/c6-3-4-1-2-5(7)8-4/h4H,1-3H2
InchiKey: HPLJEKXDAFHJPD-UHFFFAOYSA-N
Formula: C5H7ClO2
SMILES: O=C1CCC(CCl)O1
Mol. weight [g/mol]: 134.56
CAS: 39928-72-8

Physical Properties

Property code	Value	Unit	Source
gf	-192.87	kJ/mol	Joback Method
hf	-371.49	kJ/mol	Joback Method
hfus	14.33	kJ/mol	Joback Method
hvap	40.12	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	0.931		Crippen Method
mcvol	90.130	ml/mol	McGowan Method
pc	4277.45	kPa	Joback Method
tb	461.28	K	Joback Method
tc	688.12	K	Joback Method
tf	281.72	K	Joback Method
vc	0.334	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.40	J/mol×K	461.28	Joback Method
cpg	189.60	J/mol×K	499.09	Joback Method
cpg	200.29	J/mol×K	536.89	Joback Method
cpg	210.48	J/mol×K	574.70	Joback Method
cpg	220.15	J/mol×K	612.51	Joback Method
cpg	229.29	J/mol×K	650.31	Joback Method
cpg	237.90	J/mol×K	688.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39928728&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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