Oxetane, 3,3-bis-(chloromethyl)

Other names: 3,3-bis(chloromethyl)oxetane
Inchi: InChI=1S/C5H8Cl2O/c6-1-5(2-7)3-8-4-5/h1-4H2
InchiKey: CXURGFRDGROIKG-UHFFFAOYSA-N
Formula: C5H8Cl2O
SMILES: ClCC1(CCl)COC1
Mol. weight [g/mol]: 155.02
CAS: 78-71-7

Physical Properties

Property code	Value	Unit	Source
chl	-2898.30 ± 1.80	kJ/mol	NIST Webbook
gf	-75.60	kJ/mol	Joback Method
hf	-204.00 ± 1.90	kJ/mol	NIST Webbook
hfl	-260.00 ± 1.80	kJ/mol	NIST Webbook
hfus	14.82	kJ/mol	Joback Method
hvap	55.98	kJ/mol	NIST Webbook
hvap	55.98 ± 0.38	kJ/mol	NIST Webbook
hvap	56.00 ± 0.40	kJ/mol	NIST Webbook
log10ws	-0.96		Crippen Method
logp	1.481		Crippen Method
mcvol	100.800	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
rinpol	1077.00		NIST Webbook
sl	274.40	J/mol×K	NIST Webbook
tb	426.86	K	Joback Method
tc	641.95	K	Joback Method
tf	270.84	K	Joback Method
tt	292.16 ± 0.02	K	NIST Webbook
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.13	J/mol×K	426.86	Joback Method

cpg	194.95	J/mol×K	462.71	Joback Method
cpg	204.77	J/mol×K	498.56	Joback Method
cpg	213.69	J/mol×K	534.41	Joback Method
cpg	221.85	J/mol×K	570.26	Joback Method
cpg	229.35	J/mol×K	606.10	Joback Method
cpg	236.31	J/mol×K	641.95	Joback Method
cpl	218.70	J/mol×K	300.00	NIST Webbook
hfust	16.95	kJ/mol	292.20	NIST Webbook

Sources

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=C78717&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
rinpol:	Non-polar retention indices
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

vc: Critical Volume

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