Oxetane, 3,3-bis-(hydroxymethyl)

Inchi: InChI=1S/C5H10O3/c6-1-5(2-7)3-8-4-5/h6-7H,1-4H2
InchiKey: QSGREIXRTDCBHO-UHFFFAOYSA-N
Formula: C5H10O3
SMILES: OCC1(CO)COC1
Mol. weight [g/mol]: 118.13

Physical Properties

Property code	Value	Unit	Source
gf	-325.38	kJ/mol	Joback Method
hf	-501.11	kJ/mol	Joback Method
hfus	14.60	kJ/mol	Joback Method
hvap	63.53	kJ/mol	Joback Method
log10ws	0.82		Crippen Method
logp	-1.012		Crippen Method
mcvol	88.060	ml/mol	McGowan Method
pc	5713.21	kPa	Joback Method
rinpol	1200.00		NIST Webbook
tb	536.36	K	Joback Method
tc	717.15	K	Joback Method
tf	332.64	K	Joback Method
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.63	J/mol×K	536.36	Joback Method
cpg	230.51	J/mol×K	566.49	Joback Method
cpg	237.90	J/mol×K	596.62	Joback Method
cpg	244.85	J/mol×K	626.76	Joback Method
cpg	251.44	J/mol×K	656.89	Joback Method
cpg	257.74	J/mol×K	687.02	Joback Method
cpg	263.82	J/mol×K	717.15	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R6578&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume