Oxetane, 3,3-bis-(bromomethyl)

Inchi: InChI=1S/C5H8Br2O/c6-1-5(2-7)3-8-4-5/h1-4H2
InchiKey: QOPMHMFIIMJWET-UHFFFAOYSA-N
Formula: C5H8Br2O
SMILES: BrCC1(CBr)COC1
Mol. weight [g/mol]: 243.92
CAS: 2402-83-7

Physical Properties

Property code	Value	Unit	Source
gf	-23.10	kJ/mol	Joback Method
hf	-143.99	kJ/mol	Joback Method
hfus	16.99	kJ/mol	Joback Method
hvap	43.04	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	1.793		Crippen Method
mcvol	111.320	ml/mol	McGowan Method
pc	5335.72	kPa	Joback Method
tb	484.32	K	Joback Method
tc	723.65	K	Joback Method
tf	330.60	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.77	J/mol×K	484.32	Joback Method
cpg	213.96	J/mol×K	524.21	Joback Method
cpg	223.08	J/mol×K	564.10	Joback Method
cpg	231.30	J/mol×K	603.99	Joback Method
cpg	238.82	J/mol×K	643.87	Joback Method
cpg	245.81	J/mol×K	683.76	Joback Method
cpg	252.46	J/mol×K	723.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2402837&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