Alpha-(2-bromoethyl)-gamma-hydroxy butyric acid lactone

Inchi: InChI=1S/C6H9BrO2/c7-3-1-5-2-4-9-6(5)8/h5H,1-4H2
InchiKey: IGLXGNWTGHUHHI-UHFFFAOYSA-N
Formula: C6H9BrO2
SMILES: O=C1OCCC1CCBr
Mol. weight [g/mol]: 193.04
CAS: 81478-17-3

Physical Properties

Property code	Value	Unit	Source
gf	-158.20	kJ/mol	Joback Method
hf	-350.06	kJ/mol	Joback Method
hfus	18.00	kJ/mol	Joback Method
hvap	44.40	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	1.334		Crippen Method
mcvol	109.480	ml/mol	McGowan Method
pc	4333.96	kPa	Joback Method
tb	512.89	K	Joback Method
tc	747.12	K	Joback Method
tf	322.87	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.05	J/mol×K	512.89	Joback Method
cpg	242.67	J/mol×K	551.93	Joback Method
cpg	254.62	J/mol×K	590.97	Joback Method
cpg	265.89	J/mol×K	630.01	Joback Method
cpg	276.48	J/mol×K	669.05	Joback Method
cpg	286.41	J/mol×K	708.09	Joback Method
cpg	295.67	J/mol×K	747.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81478173&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

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