2(2-Bromoethyl)-1,3-dioxane

Other names: 1,3-Dioxane, 2-(2-bromoethyl)-
Inchi: InChI=1S/C6H11BrO2/c7-3-2-6-8-4-1-5-9-6/h6H,1-5H2
InchiKey: WMDHQEHPOVOEOG-UHFFFAOYSA-N
Formula: C6H11BrO2
SMILES: BrCCC1OCCCO1
Mol. weight [g/mol]: 195.05
CAS: 33884-43-4

Physical Properties

Property code	Value	Unit	Source
gf	-133.83	kJ/mol	Joback Method
hf	-350.52	kJ/mol	Joback Method
hfus	24.37	kJ/mol	Joback Method
hvap	44.83	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.534		Crippen Method
mcvol	113.780	ml/mol	McGowan Method
pc	4227.54	kPa	Joback Method
tb	476.29	K	Joback Method
tc	700.22	K	Joback Method
tf	277.70	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.88	J/mol×K	476.29	Joback Method
cpg	247.65	J/mol×K	513.61	Joback Method
cpg	260.59	J/mol×K	550.93	Joback Method
cpg	272.75	J/mol×K	588.25	Joback Method
cpg	284.14	J/mol×K	625.58	Joback Method
cpg	294.79	J/mol×K	662.90	Joback Method
cpg	304.73	J/mol×K	700.22	Joback Method
dvisc	0.0057735	Pa×s	277.70	Joback Method

dvisc	0.0029645	Pa×s	310.80	Joback Method
dvisc	0.0017305	Pa×s	343.90	Joback Method
dvisc	0.0011104	Pa×s	377.00	Joback Method
dvisc	0.0007653	Pa×s	410.09	Joback Method
dvisc	0.0005577	Pa×s	443.19	Joback Method
dvisc	0.0004246	Pa×s	476.29	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=C33884434&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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