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

Other names: 1,3-Dioxolane, 2-(2-bromoethyl)-
Inchi: InChI=1S/C5H9BrO2/c6-2-1-5-7-3-4-8-5/h5H,1-4H2
InchiKey: GGZQLTVZPOGLCC-UHFFFAOYSA-N
Formula: C5H9BrO2
SMILES: BrCCC1OCCO1
Mol. weight [g/mol]: 181.03
CAS: 18742-02-4

Physical Properties

Property code	Value	Unit	Source
gf	-130.15	kJ/mol	Joback Method
hf	-323.72	kJ/mol	Joback Method
hfus	23.88	kJ/mol	Joback Method
hvap	42.44	kJ/mol	Joback Method
log10ws	-1.02		Crippen Method
logp	1.144		Crippen Method
mcvol	99.690	ml/mol	McGowan Method
pc	4646.65	kPa	Joback Method
tb	449.14	K	Joback Method
tc	667.66	K	Joback Method
tf	269.95	K	Joback Method
vc	0.360	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.26	J/mol×K	449.14	Joback Method
cpg	205.89	J/mol×K	485.56	Joback Method
cpg	216.81	J/mol×K	521.98	Joback Method
cpg	227.06	J/mol×K	558.40	Joback Method
cpg	236.66	J/mol×K	594.82	Joback Method
cpg	245.64	J/mol×K	631.24	Joback Method
cpg	254.03	J/mol×K	667.66	Joback Method
dvisc	0.0045591	Pa×s	269.95	Joback Method

dvisc	0.0026891	Pa×s	299.81	Joback Method
dvisc	0.0017453	Pa×s	329.68	Joback Method
dvisc	0.0012171	Pa×s	359.54	Joback Method
dvisc	0.0008970	Pa×s	389.41	Joback Method
dvisc	0.0006905	Pa×s	419.27	Joback Method
dvisc	0.0005503	Pa×s	449.14	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	342.20	K	1.00	NIST Webbook

Sources

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=C18742024&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume