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]: 195.06

Physical Properties

Property code	Value	Unit	Source
hf	-387.72	kJ/mol	Cheméo Relay (1.0)
hfus	24.37	kJ/mol	Joback Method
hvap	55.11	kJ/mol	Cheméo Relay (1.0)
logp	1.534		Crippen Method
mcvol	113.780	ml/mol	McGowan 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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	341.70	K	0.40	NIST Webbook
tbrp	343.00	K	0.40	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33884434&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tbrp: Boiling point at reduced pressure

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