2-BROMOMETHYL-1,3-DIOXOLANE

Other names: 1,3-Dioxolane, 2-(bromomethyl)-
Inchi: InChI=1S/C4H7BrO2/c5-3-4-6-1-2-7-4/h4H,1-3H2
InchiKey: CKIIJIDEWWXQEA-UHFFFAOYSA-N
Formula: C4H7BrO2
SMILES: BrCC1OCCO1
Mol. weight [g/mol]: 167.00

Physical Properties

Property code	Value	Unit	Source
hfus	21.29	kJ/mol	Joback Method
ie	10.15	eV	Cheméo Relay (1.0)
logp	0.754		Crippen Method
mcvol	85.600	ml/mol	McGowan Method
tb	437.65	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.95	J/mol×K	426.26	Joback Method
cpg	166.22	J/mol×K	463.18	Joback Method
cpg	175.85	J/mol×K	500.11	Joback Method
cpg	184.87	J/mol×K	537.03	Joback Method
cpg	193.29	J/mol×K	573.96	Joback Method
cpg	201.16	J/mol×K	610.88	Joback Method
cpg	208.49	J/mol×K	647.81	Joback Method
dvisc	0.0044924	Pa×s	258.68	Joback Method
dvisc	0.0027153	Pa×s	286.61	Joback Method
dvisc	0.0017947	Pa×s	314.54	Joback Method
dvisc	0.0012691	Pa×s	342.47	Joback Method
dvisc	0.0009456	Pa×s	370.40	Joback Method
dvisc	0.0007342	Pa×s	398.33	Joback Method
dvisc	0.0005893	Pa×s	426.26	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	354.20	K	3.60	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4360638&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

hfus: Enthalpy of fusion at standard conditions

ie: Ionization energy

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tb: Normal Boiling Point Temperature

tbrp: Boiling point at reduced pressure