

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:	CKIJIJIDEWVWXQEA-UHFFFAOYSA-N
Formula:	C4H7BrO2
SMILES:	BrCC1OCCO1
Mol. weight [g/mol]:	167.00
CAS:	4360-63-8

Physical Properties

Property code	Value	Unit	Source
gf	-138.57	kJ/mol	Joback Method
hf	-303.08	kJ/mol	Joback Method
hfus	21.29	kJ/mol	Joback Method
hvap	40.21	kJ/mol	Joback Method
log10ws	-0.60		Crippen Method
logp	0.754		Crippen Method
mcvol	85.600	ml/mol	McGowan Method
pc	5320.16	kPa	Joback Method
tb	426.26	K	Joback Method
tc	647.81	K	Joback Method
tf	258.68	K	Joback Method
vc	0.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.95	J/molxK	426.26	Joback Method
cpg	201.16	J/molxK	610.88	Joback Method
cpg	193.29	J/molxK	573.96	Joback Method
cpg	184.87	J/molxK	537.03	Joback Method
cpg	175.85	J/molxK	500.11	Joback Method
cpg	166.22	J/molxK	463.18	Joback Method
cpg	208.49	J/molxK	647.81	Joback Method
dvisc	0.0005893	Paxs	426.26	Joback Method

dvisc	0.0007342	Paxs	398.33	Joback Method
dvisc	0.0009456	Paxs	370.40	Joback Method
dvisc	0.0012691	Paxs	342.47	Joback Method
dvisc	0.0017947	Paxs	314.54	Joback Method
dvisc	0.0027153	Paxs	286.61	Joback Method
dvisc	0.0044924	Paxs	258.68	Joback Method

Pressure Dependent Properties

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

Sources

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=C4360638&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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