

1,3-Dioxolane, 2-(bromomethyl)-4-methyl-, trans-

Inchi:	InChI=1S/C5H9BrO2/c1-4-3-7-5(2-6)8-4/h4-5H,2-3H2,1H3/t4-,5-/m0/s1
InchiKey:	DUQGHFJLJLUFMA-WHFBIAKZSA-N
Formula:	C5H9BrO2
SMILES:	CC1COC(CBr)O1
Mol. weight [g/mol]:	181.03
CAS:	26563-79-1

Physical Properties

Property code	Value	Unit	Source
gf	-137.86	kJ/mol	Joback Method
hf	-344.06	kJ/mol	Joback Method
hfus	24.96	kJ/mol	Joback Method
hvap	42.13	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	1.143		Crippen Method
mcvol	99.690	ml/mol	McGowan Method
pc	4444.44	kPa	Joback Method
tb	444.47	K	Joback Method
tc	662.67	K	Joback Method
tf	265.71	K	Joback Method
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.35	J/mol×K	444.47	Joback Method
cpg	207.30	J/mol×K	480.84	Joback Method
cpg	218.58	J/mol×K	517.20	Joback Method
cpg	229.21	J/mol×K	553.57	Joback Method
cpg	239.21	J/mol×K	589.93	Joback Method
cpg	248.61	J/mol×K	626.30	Joback Method
cpg	257.43	J/mol×K	662.67	Joback Method
dvisc	0.0033152	Pa×s	265.71	Joback Method
dvisc	0.0021163	Pa×s	295.50	Joback Method

dvisc	0.0014667	Pa×s	325.30	Joback Method
dvisc	0.0010810	Pa×s	355.09	Joback Method
dvisc	0.0008353	Pa×s	384.88	Joback Method
dvisc	0.0006698	Pa×s	414.68	Joback Method
dvisc	0.0005532	Pa×s	444.47	Joback Method

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=C26563791&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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