

cis-2-Bromomethyl-4-methyl-1,3-dioxolane

Inchi:	InChI=1S/C5H9BrO2/c1-4-3-7-5(2-6)8-4/h4-5H,2-3H2,1H3/t4-,5+/m0/s1
InchiKey:	DUQGHFJLJLUFMA-CRCLSJGQSA-N
Formula:	C5H9BrO2
SMILES:	CC1COC(CBr)O1
Mol. weight [g/mol]:	181.03
CAS:	26563-78-0

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/molxK	444.47	Joback Method
cpg	207.30	J/molxK	480.84	Joback Method
cpg	218.58	J/molxK	517.20	Joback Method
cpg	229.21	J/molxK	553.57	Joback Method
cpg	239.21	J/molxK	589.93	Joback Method
cpg	248.61	J/molxK	626.30	Joback Method
cpg	257.43	J/molxK	662.67	Joback Method
dvisc	0.0033152	Paxs	265.71	Joback Method
dvisc	0.0021163	Paxs	295.50	Joback Method

dvisc	0.0014667	Paxs	325.30	Joback Method
dvisc	0.0010810	Paxs	355.09	Joback Method
dvisc	0.0008353	Paxs	384.88	Joback Method
dvisc	0.0006698	Paxs	414.68	Joback Method
dvisc	0.0005532	Paxs	444.47	Joback Method

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=C26563780&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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