2-Propenal, 3-(1,3-benzodioxol-5-yl)-

Other names:	3-(1,3-benzodioxol-5-yl)acrylaldehyde
	(E)-3-(Benzo[d][1,3]dioxol-5-yl)acrylaldehyde
Inchi:	InChI=1S/C10H8O3/c11-5-1-2-8-3-4-9-10(6-8)13-7-12-9/h1-6H,7H2/b2-1+
InchiKey:	HZUFMSJUNLSDSZ-OWOJBTEDSA-N
Formula:	C10H8O3
SMILES:	O=CC=Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	176.17
CAS:	14756-00-4

Physical Properties

Property code	Value	Unit	Source
gf	3.39	kJ/mol	Joback Method
hf	-175.36	kJ/mol	Joback Method
hfus	30.43	kJ/mol	Joback Method
hvap	57.37	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.627		Crippen Method
mcvol	126.150	ml/mol	McGowan Method
pc	3877.12	kPa	Joback Method
rinpol	1648.00		NIST Webbook
rinpol	1559.10		NIST Webbook
rinpol	1559.10		NIST Webbook
tb	582.97	K	Joback Method
tc	817.27	K	Joback Method
tf	366.16	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.74	J/mol×K	582.97	Joback Method
cpg	307.99	J/mol×K	622.02	Joback Method
cpg	318.33	J/mol×K	661.07	Joback Method
cpg	327.86	J/mol×K	700.12	Joback Method

cpg	336.65	J/mol×K	739.17	Joback Method
cpg	344.80	J/mol×K	778.22	Joback Method
cpg	352.39	J/mol×K	817.27	Joback Method
dvisc	0.0022365	Pa×s	366.16	Joback Method
dvisc	0.0015339	Pa×s	402.30	Joback Method
dvisc	0.0011194	Pa×s	438.43	Joback Method
dvisc	0.0008571	Pa×s	474.57	Joback Method
dvisc	0.0006815	Pa×s	510.70	Joback Method
dvisc	0.0005586	Pa×s	546.84	Joback Method
dvisc	0.0004693	Pa×s	582.97	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=C14756004&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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