3-(Benzo[d][1,3]dioxol-5-yl)propanal

Other names: 3-(Benzo[d][1,3]dioxol-5-yl)propanal
Inchi: InChI=1S/C10H10O3/c11-5-1-2-8-3-4-9-10(6-8)13-7-12-9/h3-6H,1-2,7H2
InchiKey: IDCKZBGINKOTOL-UHFFFAOYSA-N
Formula: C10H10O3
SMILES: O=CCCc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 178.19

Physical Properties

Property code	Value	Unit	Source
hfus	30.23	kJ/mol	Joback Method
hvap	69.05	kJ/mol	Cheméo Relay (1.0)
ie	8.19	eV	Cheméo Relay (1.0)
log10ws	-1.92		Cheméo Relay (1.0)
logp	1.547		Crippen Method
mcvol	130.450	ml/mol	McGowan Method
tb	548.34	K	Cheméo Relay (1.0)
tf	294.07	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.97	J/mol×K	578.81	Joback Method
cpg	377.27	J/mol×K	802.91	Joback Method
cpg	368.94	J/mol×K	765.56	Joback Method
cpg	360.01	J/mol×K	728.21	Joback Method
cpg	350.40	J/mol×K	690.86	Joback Method
cpg	340.07	J/mol×K	653.51	Joback Method
cpg	328.94	J/mol×K	616.16	Joback Method
dvisc	0.0009901	Pa×s	475.03	Joback Method
dvisc	0.0005492	Pa×s	578.81	Joback Method
dvisc	0.0006520	Pa×s	544.22	Joback Method
dvisc	0.0007921	Pa×s	509.62	Joback Method
dvisc	0.0024815	Pa×s	371.24	Joback Method
dvisc	0.0012817	Pa×s	440.43	Joback Method

dvisc	0.0017339	Pa×s	405.84	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30830558&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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point