6,7-Dimethoxy-2H-1,3-benzodioxole-5-carbaldehy

Other names: 6,7-Dimethoxybenzo[d][1,3]dioxole-5-carbaldehyde
Inchi: InChI=1S/C10H10O5/c1-12-8-6(4-11)3-7-9(10(8)13-2)15-5-14-7/h3-4H,5H2,1-2H3
InchiKey: GWFYXQGVKQUWFF-UHFFFAOYSA-N
Formula: C10H10O5
SMILES: COc1c(C=O)cc2c(c1OC)OCO2
Mol. weight [g/mol]: 210.18
CAS: 23731-65-9

Physical Properties

Property code	Value	Unit	Source
gf	-306.09	kJ/mol	Joback Method
hf	-579.96	kJ/mol	Joback Method
hfus	31.83	kJ/mol	Joback Method
hvap	63.56	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	1.245		Crippen Method
mcvol	142.190	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	1628.70		NIST Webbook
rinpol	1628.70		NIST Webbook
tb	633.61	K	Joback Method
tc	853.92	K	Joback Method
tf	440.74	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.78	J/mol×K	633.61	Joback Method
cpg	371.93	J/mol×K	670.33	Joback Method
cpg	382.44	J/mol×K	707.05	Joback Method
cpg	392.31	J/mol×K	743.76	Joback Method
cpg	401.56	J/mol×K	780.48	Joback Method
cpg	410.20	J/mol×K	817.20	Joback Method

cpg	418.24	J/mol×K	853.92	Joback Method
dvisc	0.0011599	Pa×s	440.74	Joback Method
dvisc	0.0008920	Pa×s	472.88	Joback Method
dvisc	0.0007093	Pa×s	505.03	Joback Method
dvisc	0.0005797	Pa×s	537.17	Joback Method
dvisc	0.0004847	Pa×s	569.32	Joback Method
dvisc	0.0004131	Pa×s	601.47	Joback Method
dvisc	0.0003578	Pa×s	633.61	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C23731659&Units=SI

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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