1,3-benzodioxole-5-propionaldehyde

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]: 178.18
CAS: 30830-55-8

Physical Properties

Property code	Value	Unit	Source
gf	-76.83	kJ/mol	Joback Method
hf	-292.58	kJ/mol	Joback Method
hfus	30.23	kJ/mol	Joback Method
hvap	57.42	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.547		Crippen Method
mcvol	130.450	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
rinpol	1522.90		NIST Webbook
rinpol	1522.90		NIST Webbook
tb	578.81	K	Joback Method
tc	802.91	K	Joback Method
tf	371.24	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.97	J/mol×K	578.81	Joback Method
cpg	328.94	J/mol×K	616.16	Joback Method
cpg	340.07	J/mol×K	653.51	Joback Method
cpg	350.40	J/mol×K	690.86	Joback Method
cpg	360.01	J/mol×K	728.21	Joback Method
cpg	368.94	J/mol×K	765.56	Joback Method

cpg	377.27	J/mol×K	802.91	Joback Method
dvisc	0.0024815	Pa×s	371.24	Joback Method
dvisc	0.0017339	Pa×s	405.83	Joback Method
dvisc	0.0012817	Pa×s	440.43	Joback Method
dvisc	0.0009901	Pa×s	475.02	Joback Method
dvisc	0.0007921	Pa×s	509.62	Joback Method
dvisc	0.0006520	Pa×s	544.21	Joback Method
dvisc	0.0005492	Pa×s	578.81	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=C30830558&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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