

p-Propionoxybenzaldehyde

Other names:	4-n-Propionyloxybenzaldehyde Benzaldehyde, 4-(1-oxopropoxy)-
Inchi:	InChI=1S/C10H10O3/c1-2-10(12)13-9-5-3-8(7-11)4-6-9/h3-7H,2H2,1H3
InchiKey:	NKXPJXVTMWLHBC-UHFFFAOYSA-N
Formula:	C10H10O3
SMILES:	CCC(=O)Oc1ccc(C=O)cc1
Mol. weight [g/mol]:	178.18
CAS:	50262-48-1

Physical Properties

Property code	Value	Unit	Source
gf	-197.34	kJ/mol	Joback Method
hf	-355.05	kJ/mol	Joback Method
hfus	20.38	kJ/mol	Joback Method
hvap	56.67	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	1.814		Crippen Method
mcvol	137.010	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
tb	584.81	K	Joback Method
tc	801.61	K	Joback Method
tf	355.56	K	Joback Method
vc	0.528	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.66	J/mol×K	584.81	Joback Method
cpg	368.64	J/mol×K	765.48	Joback Method
cpg	359.60	J/mol×K	729.34	Joback Method
cpg	349.89	J/mol×K	693.21	Joback Method
cpg	339.51	J/mol×K	657.08	Joback Method
cpg	328.43	J/mol×K	620.94	Joback Method
cpg	377.02	J/mol×K	801.61	Joback Method

dvisc	0.0002484	Paxs	584.81	Joback Method
dvisc	0.0003078	Paxs	546.60	Joback Method
dvisc	0.0003940	Paxs	508.39	Joback Method
dvisc	0.0005249	Paxs	470.18	Joback Method
dvisc	0.0007358	Paxs	431.98	Joback Method
dvisc	0.0011012	Paxs	393.77	Joback Method
dvisc	0.0017973	Paxs	355.56	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	406.50 ± 2.50	K	0.07	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50262481&Units=SI
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

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
tbrp:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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