

p-Isopropenylbenzaldehyde

Inchi:	InChI=1S/C10H10O/c1-8(2)10-5-3-9(7-11)4-6-10/h3-7H,1H2,2H3
InchiKey:	IRWAASJGTLXGMV-UHFFFAOYSA-N
Formula:	C10H10O
SMILES:	<chem>C=C(C)c1ccc(C=O)cc1</chem>
Mol. weight [g/mol]:	146.19

Physical Properties

Property code	Value	Unit	Source
gf	115.87	kJ/mol	Joback Method
hf	5.39	kJ/mol	Joback Method
hfus	15.01	kJ/mol	Joback Method
hvap	46.92	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.532		Crippen Method
mvol	125.270	ml/mol	McGowan Method
pc	3299.15	kPa	Joback Method
ripol	1957.00		NIST Webbook
tb	505.08	K	Joback Method
tc	724.63	K	Joback Method
tf	267.68	K	Joback Method
vc	0.486	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.70	J/mol×K	505.08	Joback Method
cpg	272.39	J/mol×K	541.67	Joback Method
cpg	284.29	J/mol×K	578.26	Joback Method
cpg	295.42	J/mol×K	614.85	Joback Method
cpg	305.82	J/mol×K	651.44	Joback Method
cpg	315.54	J/mol×K	688.04	Joback Method
cpg	324.61	J/mol×K	724.63	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=R325563&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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