3-Isopropylbenzaldehyde

Other names: Benzaldehyde, 3-(1-methylethyl)-
Inchi: InChI=1S/C10H12O/c1-8(2)10-5-3-4-9(6-10)7-11/h3-8H,1-2H3
InchiKey: FFQXEFNKZVGJDI-UHFFFAOYSA-N
Formula: C10H12O
SMILES: CC(C)c1cccc(C=O)c1
Mol. weight [g/mol]: 148.20
CAS: 34246-57-6

Physical Properties

Property code	Value	Unit	Source
gf	34.14	kJ/mol	Joback Method
hf	-115.53	kJ/mol	Joback Method
hfus	14.07	kJ/mol	Joback Method
hvap	47.12	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.623		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
rinpol	1234.00		NIST Webbook
tb	508.08	K	Joback Method
tc	723.60	K	Joback Method
tf	268.40	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.08	J/mol×K	508.08	Joback Method
cpg	291.66	J/mol×K	544.00	Joback Method
cpg	304.45	J/mol×K	579.92	Joback Method
cpg	316.47	J/mol×K	615.84	Joback Method
cpg	327.76	J/mol×K	651.76	Joback Method
cpg	338.34	J/mol×K	687.68	Joback Method
cpg	348.24	J/mol×K	723.60	Joback Method

dvisc	0.0033646	Pa×s	268.40	Joback Method
dvisc	0.0016592	Pa×s	308.35	Joback Method
dvisc	0.0009623	Pa×s	348.29	Joback Method
dvisc	0.0006243	Pa×s	388.24	Joback Method
dvisc	0.0004391	Pa×s	428.19	Joback Method
dvisc	0.0003279	Pa×s	468.13	Joback Method
dvisc	0.0002564	Pa×s	508.08	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=C34246576&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