

Benzaldehyde, 4-(1-methylethyl)-

Other names:	4-(1-Methylethyl)benzaldehyde 4-Isopropylbenzaldehyde 4-Isopropylphenylcarboxaldehyde 4-iPr-Benzaldehyde Benzaldehyde, p-isopropyl- Cumal Cumaldehyde Cumic aldehyde Cuminal Cuminaldehyde Cuminic aldehyde Cuminyl aldehyde NSC 4886 p-(1-methylethyl)benzaldehyde p-Cumic aldehyde p-Cuminic aldehyde p-Isopropylbenzaldehyde p-Isopropylbenzenecarboxaldehyde
Inchi:	InChI=1S/C10H12O/c1-8(2)10-5-3-9(7-11)4-6-10/h3-8H,1-2H3
InchiKey:	WTWBUQJHJGUZCY-UHFFFAOYSA-N
Formula:	C10H12O
SMILES:	CC(C)c1ccc(C=O)cc1
Mol. weight [g/mol]:	148.20
CAS:	122-03-2

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
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tb	508.65 ± 1.00	K	NIST Webbook
tb	508.70	K	NIST Webbook
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	348.24	J/mol×K	723.60	Joback Method
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
dvisc	0.0002564	Pa×s	508.08	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
hvapt	55.30	kJ/mol	418.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.70	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.57194e+01
Coeff. B	-5.20755e+03
Coeff. C	-3.95980e+01
Temperature range (K), min.	377.05
Temperature range (K), max.	539.94

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=C122032&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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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