

4-(t-Butoxy)benzaldehyde

Other names:	Benzaldehyde, 4-(1,1-dimethylethoxy)- 4-(Tert-butoxy)benzaldehyde p-tert-butoxybenzaldehyde
Inchi:	InChI=1S/C11H14O2/c1-11(2,3)13-10-6-4-9(8-12)5-7-10/h4-8H,1-3H3
InchiKey:	VWSFZYXXQDKXKQ-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CC(C)(C)Oc1ccc(C=O)cc1
Mol. weight [g/mol]:	178.23
CAS:	57699-45-3

Physical Properties

Property code	Value	Unit	Source
gf	-57.16	kJ/mol	Joback Method
hf	-271.86	kJ/mol	Joback Method
hfus	13.96	kJ/mol	Joback Method
hvap	50.85	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.676		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
tb	550.59	K	Joback Method
tc	768.91	K	Joback Method
tf	319.32	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.38	J/molxK	550.59	Joback Method
cpg	365.11	J/molxK	586.98	Joback Method
cpg	378.90	J/molxK	623.36	Joback Method
cpg	391.79	J/molxK	659.75	Joback Method
cpg	403.83	J/molxK	696.14	Joback Method
cpg	415.04	J/molxK	732.53	Joback Method

cpg	425.47	J/mol×K	768.91	Joback Method
dvisc	0.0023506	Paxs	319.32	Joback Method
dvisc	0.0012452	Paxs	357.87	Joback Method
dvisc	0.0007464	Paxs	396.41	Joback Method
dvisc	0.0004899	Paxs	434.95	Joback Method
dvisc	0.0003444	Paxs	473.50	Joback Method
dvisc	0.0002552	Paxs	512.04	Joback Method
dvisc	0.0001973	Paxs	550.59	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=C57699453&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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