4-tert-butylbenzaldehyde

Inchi: InChI=1S/C11H14O/c1-11(2,3)10-6-4-9(8-12)5-7-10/h4-8H,1-3H3
InchiKey: OTXINXDGSUFPNU-UHFFFAOYSA-N
Formula: C11H14O
SMILES: CC(C)(C)c1ccc(C=O)cc1
Mol. weight [g/mol]: 162.23

Physical Properties

Property code	Value	Unit	Source
gf	47.84	kJ/mol	Joback Method
hf	-139.64	kJ/mol	Joback Method
hfus	12.77	kJ/mol	Joback Method
hvap	48.44	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.797		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
tb	528.17	K	Joback Method
tc	749.05	K	Joback Method
tf	297.09	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.80	J/mol×K	528.17	Joback Method
cpg	391.89	J/mol×K	712.24	Joback Method
cpg	380.51	J/mol×K	675.43	Joback Method
cpg	368.27	J/mol×K	638.61	Joback Method
cpg	355.11	J/mol×K	601.80	Joback Method
cpg	340.98	J/mol×K	564.98	Joback Method
cpg	402.46	J/mol×K	749.05	Joback Method
dvisc	0.0002424	Pa×s	528.17	Joback Method
dvisc	0.0003151	Pa×s	489.66	Joback Method
dvisc	0.0004284	Pa×s	451.14	Joback Method

dvisc	0.0006168	Pa×s	412.63	Joback Method
dvisc	0.0009572	Pa×s	374.12	Joback Method
dvisc	0.0016432	Pa×s	335.60	Joback Method
dvisc	0.0032448	Pa×s	297.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=T999909250&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume