2,3,6-Trimethylbenzaldehyde

Other names: 2,3,6-trimethylbenzadehyde
Inchi: InChI=1S/C10H12O/c1-7-4-5-8(2)10(6-11)9(7)3/h4-6H,1-3H3
InchiKey: NHMDCMLCZRILTI-UHFFFAOYSA-N
Formula: C10H12O
SMILES: Cc1ccc(C)c(C=O)c1C
Mol. weight [g/mol]: 148.20
CAS: 34341-29-2

Physical Properties

Property code	Value	Unit	Source
gf	17.32	kJ/mol	Joback Method
hf	-133.19	kJ/mol	Joback Method
hfus	16.82	kJ/mol	Joback Method
hvap	48.84	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.424		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
tb	518.48	K	Joback Method
tc	731.53	K	Joback Method
tf	308.44	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.66	J/mol×K	518.48	Joback Method
cpg	290.15	J/mol×K	553.99	Joback Method
cpg	302.00	J/mol×K	589.50	Joback Method
cpg	313.24	J/mol×K	625.00	Joback Method
cpg	323.88	J/mol×K	660.51	Joback Method
cpg	333.94	J/mol×K	696.02	Joback Method
cpg	343.43	J/mol×K	731.53	Joback Method
dvisc	0.0014505	Pa×s	308.44	Joback Method

dvisc	0.0009364	Pa×s	343.45	Joback Method
dvisc	0.0006555	Pa×s	378.45	Joback Method
dvisc	0.0004874	Pa×s	413.46	Joback Method
dvisc	0.0003796	Pa×s	448.47	Joback Method
dvisc	0.0003065	Pa×s	483.47	Joback Method
dvisc	0.0002548	Pa×s	518.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34341292&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