Benzaldehyde, 3,5-dimethyl-

Inchi: InChI=1S/C9H10O/c1-7-3-8(2)5-9(4-7)6-10/h3-6H,1-2H3
InchiKey: NBEFMISJJNGCIZ-UHFFFAOYSA-N
Formula: C9H10O
SMILES: Cc1cc(C)cc(C=O)c1
Mol. weight [g/mol]: 134.18
CAS: 5779-95-3

Physical Properties

Property code	Value	Unit	Source
gf	18.53	kJ/mol	Joback Method
hf	-101.08	kJ/mol	Joback Method
hfus	14.62	kJ/mol	Joback Method
hvap	45.95	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.116		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	1169.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1169.00		NIST Webbook
ripol	1837.00		NIST Webbook
tb	490.62	K	Joback Method
tc	705.85	K	Joback Method
tf	284.65	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.09	J/mol×K	490.62	Joback Method
cpg	287.67	J/mol×K	669.98	Joback Method
cpg	278.35	J/mol×K	634.11	Joback Method
cpg	268.44	J/mol×K	598.24	Joback Method
cpg	257.95	J/mol×K	562.36	Joback Method

cpg	246.84	J/mol×K	526.49	Joback Method
cpg	296.44	J/mol×K	705.85	Joback Method
dvisc	0.0002714	Pa×s	490.62	Joback Method
dvisc	0.0003303	Pa×s	456.29	Joback Method
dvisc	0.0004151	Pa×s	421.96	Joback Method
dvisc	0.0005432	Pa×s	387.63	Joback Method
dvisc	0.0007489	Pa×s	353.31	Joback Method
dvisc	0.0011064	Pa×s	318.98	Joback Method
dvisc	0.0017961	Pa×s	284.65	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5779953&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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Latest version available from: