3,5-Dimethylbenzaldehyde

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

Physical Properties

Property code	Value	Unit	Source
af	0.4574		Cheméo Relay (1.0)
gf	18.53	kJ/mol	Joback Method
hf	-111.95	kJ/mol	Cheméo Relay (1.0)
hfus	14.62	kJ/mol	Joback Method
ie	9.13	eV	Cheméo Relay (1.0)
log10ws	-2.08		Cheméo Relay (1.0)
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	495.77	K	Cheméo Relay (1.0)
tc	729.22	K	Cheméo Relay (1.0)
tf	262.78	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.09	J/mol×K	490.62	Joback Method
cpg	296.44	J/mol×K	705.85	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
dvisc	0.0005432	Pa×s	387.63	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	0.0017961	Pa×s	284.65	Joback Method
dvisc	0.0007489	Pa×s	353.31	Joback Method
dvisc	0.0011064	Pa×s	318.98	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5779953&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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