Benzaldehyde dimethyl acetal

Other names:	Benzene, (dimethoxymethyl)- «alpha»,«alpha»-Dimethoxytoluene Dimethoxymethylbenzene Dimethoxyphenylmethane Toluene, «alpha»,«alpha»-dimethoxy- alpha,alpha-dimethoxytoluene
Inchi:	InChI=1S/C9H12O2/c1-10-9(11-2)8-6-4-3-5-7-8/h3-7,9H,1-2H3
InchiKey:	HEVMDQBCAHEHDY-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	COC(OC)c1ccccc1
Mol. weight [g/mol]:	152.19
CAS:	1125-88-8

Physical Properties

Property code	Value	Unit	Source
chl	-4948.16 ± 0.47	kJ/mol	NIST Webbook
gf	-75.13	kJ/mol	Joback Method
hf	-248.94 ± 0.88	kJ/mol	NIST Webbook
hfl	-308.40 ± 0.52	kJ/mol	NIST Webbook
hfus	11.96	kJ/mol	Joback Method
hvap	59.50	kJ/mol	NIST Webbook
hvap	60.90 ± 0.50	kJ/mol	NIST Webbook
hvap	59.46 ± 0.71	kJ/mol	NIST Webbook
log10ws	-1.82		Crippen Method
logp	1.978		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	1200.00		NIST Webbook
ripol	1665.00		NIST Webbook
tb	469.00	K	NIST Webbook
tb	480.00 ± 5.00	K	NIST Webbook
tc	685.46	K	Joback Method
tf	247.07	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.07	J/mol×K	685.46	Joback Method
cpg	262.36	J/mol×K	476.40	Joback Method
cpg	276.05	J/mol×K	511.24	Joback Method
cpg	289.11	J/mol×K	546.09	Joback Method
cpg	301.54	J/mol×K	580.93	Joback Method
cpg	313.34	J/mol×K	615.77	Joback Method
cpg	324.51	J/mol×K	650.62	Joback Method
dvisc	0.0001657	Pa×s	476.40	Joback Method
dvisc	0.0029241	Pa×s	247.07	Joback Method
dvisc	0.0013153	Pa×s	285.29	Joback Method
dvisc	0.0007146	Pa×s	323.51	Joback Method
dvisc	0.0004417	Pa×s	361.74	Joback Method
dvisc	0.0002993	Pa×s	399.96	Joback Method
dvisc	0.0002170	Pa×s	438.18	Joback Method
hvapt	56.50 ± 0.70	kJ/mol	300.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	361.20	K	2.40	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1125888&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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume