

Benzenemethanol, 3,4,5-trimethoxy-

Other names:	Benzylic alcohol, 3,4,5-trimethoxy- 3,4,5-Trimethoxybenzylic alcohol 3,4,5-trimethoxybenzylic alcohol
Inchi:	InChI=1S/C10H14O4/c1-12-8-4-7(6-11)5-9(13-2)10(8)14-3/h4-5,11H,6H2,1-3H3
InchiKey:	QPHLRCUCFDXGLY-UHFFFAOYSA-N
Formula:	C10H14O4
SMILES:	COc1cc(CO)cc(OC)c1OC
Mol. weight [g/mol]:	198.22
CAS:	3840-31-1

Physical Properties

Property code	Value	Unit	Source
gf	-334.98	kJ/mol	Joback Method
hf	-596.50	kJ/mol	Joback Method
hfus	22.18	kJ/mol	Joback Method
hvap	66.02	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	1.205		Crippen Method
mcvol	151.480	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
tb	629.26	K	Joback Method
tc	820.43	K	Joback Method
tf	393.95	K	Joback Method
vc	0.560	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.12	J/mol×K	629.26	Joback Method
cpg	393.57	J/mol×K	661.12	Joback Method
cpg	404.54	J/mol×K	692.98	Joback Method
cpg	415.01	J/mol×K	724.85	Joback Method
cpg	424.96	J/mol×K	756.71	Joback Method
cpg	434.36	J/mol×K	788.57	Joback Method

cpg	443.21	J/molxK	820.43	Joback Method
dvisc	0.0008483	Paxs	393.95	Joback Method
dvisc	0.0004050	Paxs	433.17	Joback Method
dvisc	0.0002186	Paxs	472.39	Joback Method
dvisc	0.0001297	Paxs	511.61	Joback Method
dvisc	0.0000829	Paxs	550.82	Joback Method
dvisc	0.0000562	Paxs	590.04	Joback Method
dvisc	0.0000400	Paxs	629.26	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	501.20	K	3.30	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3840311&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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