

4-ETHOXY-3-METHOXYBENZYL ALCOHOL

Other names:	Benzenemethanol, 4-ethoxy-3-methoxy-
Inchi:	InChI=1S/C10H14O3/c1-3-13-9-5-4-8(7-11)6-10(9)12-2/h4-6,11H,3,7H2,1-2H3
InchiKey:	PMSHVORCBMOTBP-UHFFFAOYSA-N
Formula:	C10H14O3
SMILES:	CCOc1ccc(CO)cc1OC
Mol. weight [g/mol]:	182.22

Physical Properties

Property code	Value	Unit	Source
hfus	21.38	kJ/mol	Joback Method
ie	7.97	eV	Cheméo Relay (1.0)
log10ws	-1.60		Cheméo Relay (1.0)
logp	1.586		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
tb	553.34	K	Cheméo Relay (1.0)
tf	339.56	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.82	J/mol×K	601.86	Joback Method
cpg	370.51	J/mol×K	633.78	Joback Method
cpg	381.67	J/mol×K	665.71	Joback Method
cpg	392.30	J/mol×K	697.63	Joback Method
cpg	402.40	J/mol×K	729.56	Joback Method
cpg	411.97	J/mol×K	761.48	Joback Method
cpg	421.01	J/mol×K	793.40	Joback Method
dvisc	0.0018895	Pa×s	359.20	Joback Method
dvisc	0.0007786	Pa×s	399.64	Joback Method
dvisc	0.0003776	Pa×s	440.09	Joback Method
dvisc	0.0002069	Pa×s	480.53	Joback Method
dvisc	0.0001244	Pa×s	520.97	Joback Method
dvisc	0.0000805	Pa×s	561.42	Joback Method
dvisc	0.0000553	Pa×s	601.86	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	459.20	K	1.00	NIST Webbook

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=C61813589&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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