

5-Ethoxy-2-hydroxy-m-xylene-alpha1,alpha3-diol

Other names:	5-Ethoxy-2-hydroxy-m-xylene-alpha
Inchi:	InChI=1S/C10H14O4/c1-2-14-9-3-7(5-11)10(13)8(4-9)6-12/h3-4,11-13H,2,5-6H2,1H3
InchiKey:	NBFKYLZEXFDQTQ-UHFFFAOYSA-N
Formula:	C10H14O4
SMILES:	CCOc1cc(CO)c(O)c(CO)c1
Mol. weight [g/mol]:	198.22

Physical Properties

Property code	Value	Unit	Source
hfus	30.07	kJ/mol	Joback Method
ie	8.03	eV	Cheméo Relay (1.0)
logp	0.776		Crippen Method
mcvol	151.480	ml/mol	McGowan Method
tb	605.38	K	Cheméo Relay (1.0)
tf	392.46	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.60	J/mol×K	752.24	Joback Method
cpg	437.63	J/mol×K	784.65	Joback Method
cpg	446.25	J/mol×K	817.07	Joback Method
cpg	454.48	J/mol×K	849.48	Joback Method
cpg	462.38	J/mol×K	881.89	Joback Method
cpg	469.98	J/mol×K	914.31	Joback Method
cpg	477.32	J/mol×K	946.72	Joback Method
dvisc	0.0000708	Pa×s	509.51	Joback Method
dvisc	0.0000248	Pa×s	549.97	Joback Method
dvisc	0.0000101	Pa×s	590.42	Joback Method
dvisc	0.0000046	Pa×s	630.88	Joback Method
dvisc	0.0000023	Pa×s	671.33	Joback Method
dvisc	0.0000012	Pa×s	711.79	Joback Method
dvisc	0.0000007	Pa×s	752.24	Joback Method

Sources

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=C131378524&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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