

BENZENEMETHANOL, .ALPHA.-(ETHOXYMETHYL)-

Other names:	«alpha»-(Ethoxymethyl)benzyl alcohol
Inchi:	InChI=1S/C10H14O2/c1-2-12-8-10(11)9-6-4-3-5-7-9/h3-7,10-11H,2,8H2,1H3
InchiKey:	XSBXONDDSWGIMG-UHFFFAOYSA-N
Formula:	C10H14O2
SMILES:	CCOCC(O)c1ccccc1
Mol. weight [g/mol]:	166.22

Physical Properties

Property code	Value	Unit	Source
af	0.6211		Cheméo Relay (1.0)
hf	-312.85	kJ/mol	Cheméo Relay (1.0)
hfus	17.45	kJ/mol	Joback Method
hvap	77.02	kJ/mol	Cheméo Relay (1.0)
ie	8.90	eV	Cheméo Relay (1.0)
log10ws	-1.05		Cheméo Relay (1.0)
logp	1.756		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
tb	509.55	K	Cheméo Relay (1.0)
tc	726.30	K	Cheméo Relay (1.0)
tf	296.13	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.30	J/mol×K	569.04	Joback Method
cpg	348.87	J/mol×K	601.51	Joback Method
cpg	360.77	J/mol×K	633.97	Joback Method
cpg	372.02	J/mol×K	666.44	Joback Method
cpg	382.64	J/mol×K	698.90	Joback Method
cpg	392.65	J/mol×K	731.37	Joback Method
cpg	402.07	J/mol×K	763.83	Joback Method
dvisc	0.0122682	Pa×s	296.93	Joback Method
dvisc	0.0029883	Pa×s	342.28	Joback Method

dvisc	0.0010130	Pa×s	387.63	Joback Method
dvisc	0.0004307	Pa×s	432.99	Joback Method
dvisc	0.0002154	Pa×s	478.34	Joback Method
dvisc	0.0001214	Pa×s	523.69	Joback Method
dvisc	0.0000750	Pa×s	569.04	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=C22383535&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

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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