1,2-Ethanediol, monobenzoate

Other names:	«beta»-Hydroxyethyl benzoate
	Ethylene glycol monobenzoate
	2-(Benzoyloxy)ethanol
	2-Hydroxyethyl benzoate
	Benzoic acid, 2-hydroxyethyl ester
Inchi:	InChI=1S/C9H10O3/c10-6-7-12-9(11)8-4-2-1-3-5-8/h1-5,10H,6-7H2
InchiKey:	LSWRBVSEWBWTDR-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	O=C(OCCO)c1ccccc1
Mol. weight [g/mol]:	166.17
CAS:	94-33-7

Physical Properties

Property code	Value	Unit	Source
gf	-233.43	kJ/mol	Joback Method
hf	-389.59	kJ/mol	Joback Method
hfus	19.98	kJ/mol	Joback Method
hvap	63.74	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	0.836		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
ripol	1780.00		NIST Webbook
ripol	1780.00		NIST Webbook
tb	600.47	K	Joback Method
tc	801.75	K	Joback Method
tf	350.59	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.10	J/mol×K	600.47	Joback Method
cpg	349.97	J/mol×K	768.21	Joback Method

cpg	341.95	J/mol×K	734.66	Joback Method
cpg	333.37	J/mol×K	701.11	Joback Method
cpg	324.21	J/mol×K	667.56	Joback Method
cpg	314.46	J/mol×K	634.02	Joback Method
cpg	357.45	J/mol×K	801.75	Joback Method
dvisc	0.0000813	Pa×s	600.47	Joback Method
dvisc	0.0001222	Pa×s	558.82	Joback Method
dvisc	0.0001960	Pa×s	517.18	Joback Method
dvisc	0.0003415	Pa×s	475.53	Joback Method
dvisc	0.0006620	Pa×s	433.88	Joback Method
dvisc	0.0014770	Pa×s	392.24	Joback Method
dvisc	0.0039872	Pa×s	350.59	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C94337&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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