

2-Propenoic acid, 4-hydroxybutyl ester

Other names:	2-Propenoic acid, 4-hydroxybutyl ester 1,4-Butanediol monoacrylate Butanediol monoacrylate
Inchi:	InChI=1S/C7H12O3/c1-2-7(9)10-6-4-3-5-8/h2,8H,1,3-6H2
InchiKey:	NDWUBGAGUCISDV-UHFFFAOYSA-N
Formula:	C7H12O3
SMILES:	C=CC(=O)OCCCCO
Mol. weight [g/mol]:	144.17

Physical Properties

Property code	Value	Unit	Source
af	0.7353		Cheméo Relay (1.0)
hf	-540.24	kJ/mol	Cheméo Relay (1.0)
hfus	19.48	kJ/mol	Joback Method
hvap	70.22	kJ/mol	Cheméo Relay (1.0)
ie	10.02	eV	Cheméo Relay (1.0)
log10ws	-0.28		Cheméo Relay (1.0)
logp	0.488		Crippen Method
mcvol	118.500	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
rinpol	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
tb	490.05	K	Cheméo Relay (1.0)
tc	692.14	K	Cheméo Relay (1.0)
tf	263.42	K	Cheméo Relay (1.0)
vc	0.429	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.97	J/mol×K	524.71	Joback Method
cpg	319.82	J/mol×K	697.39	Joback Method
cpg	312.39	J/mol×K	668.61	Joback Method

cpg	304.62	J/mol×K	639.83	Joback Method
cpg	296.50	J/mol×K	611.05	Joback Method
cpg	288.02	J/mol×K	582.27	Joback Method
cpg	279.18	J/mol×K	553.49	Joback Method
dvisc	0.0006469	Pa×s	412.29	Joback Method
dvisc	0.0001366	Pa×s	524.71	Joback Method
dvisc	0.0002118	Pa×s	487.24	Joback Method
dvisc	0.0003534	Pa×s	449.76	Joback Method
dvisc	0.0098287	Pa×s	299.87	Joback Method
dvisc	0.0013365	Pa×s	374.82	Joback Method
dvisc	0.0032441	Pa×s	337.34	Joback Method

Sources

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=C2478106&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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