2-BUTEN-1-OL, ACETATE

Other names: trans-2-Butenyl acetate
Crotyl alcohol, acetate
(2E)-2-Butenyl acetate
Inchi: InChI=1S/C6H10O2/c1-3-4-5-8-6(2)7/h3-4H,5H2,1-2H3
InchiKey: WNHXJHGRIHUOTG-ONEGZZNKSA-N
Formula: C6H10O2
SMILES: C/C=C/COC(C)=O
Mol. weight [g/mol]: 114.14

Physical Properties

Property code	Value	Unit	Source
af	0.3576		Cheméo Relay (1.0)
gf	-154.06	kJ/mol	Joback Method
hf	-372.41	kJ/mol	Cheméo Relay (1.0)
hfus	14.28	kJ/mol	Joback Method
hvap	42.41	kJ/mol	Cheméo Relay (1.0)
ie	9.15	eV	Cheméo Relay (1.0)
log10ws	-1.33		Cheméo Relay (1.0)
logp	1.126		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
rinpol	823.60		NIST Webbook
rinpol	897.00		NIST Webbook
tb	401.25	K	Cheméo Relay (1.0)
tc	576.48	K	Cheméo Relay (1.0)
tf	186.58	K	Cheméo Relay (1.0)
vc	0.354	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.29	J/mol×K	417.13	Joback Method
cpg	193.78	J/mol×K	448.23	Joback Method
cpg	202.88	J/mol×K	479.33	Joback Method

cpg	211.61	J/mol×K	510.43	Joback Method
cpg	219.98	J/mol×K	541.53	Joback Method
cpg	227.98	J/mol×K	572.63	Joback Method
cpg	235.63	J/mol×K	603.73	Joback Method
dvisc	0.0027763	Pa×s	224.46	Joback Method
dvisc	0.0014062	Pa×s	256.57	Joback Method
dvisc	0.0008286	Pa×s	288.68	Joback Method
dvisc	0.0005428	Pa×s	320.80	Joback Method
dvisc	0.0003840	Pa×s	352.91	Joback Method
dvisc	0.0002879	Pa×s	385.02	Joback Method
dvisc	0.0002255	Pa×s	417.13	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=C628080&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor

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

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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https://www.chemeo.com/cid/57-571-5/2-BUTEN-1-OL-ACETATE.pdf
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