2-methylbutyl 2-propenoate

Other names: 2-methylbutyl acrylate
Inchi: InChI=1S/C8H14O2/c1-4-7(3)6-10-8(9)5-2/h5,7H,2,4,6H2,1,3H3
InchiKey: NCTBYWFEJFTVEL-UHFFFAOYSA-N
Formula: C8H14O2
SMILES: C=CC(=O)OCC(C)CC
Mol. weight [g/mol]: 142.20
CAS: 44914-03-6

Physical Properties

Property code	Value	Unit	Source
af	0.4880		Cheméo Relay (1.0)
hf	-430.90	kJ/mol	Cheméo Relay (1.0)
hfus	14.46	kJ/mol	Joback Method
hvap	45.16	kJ/mol	Cheméo Relay (1.0)
ie	10.18	eV	Cheméo Relay (1.0)
log10ws	-2.12		Cheméo Relay (1.0)
logp	1.762		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
tb	428.67	K	Cheméo Relay (1.0)
tc	617.09	K	Cheméo Relay (1.0)
tf	195.12	K	Cheméo Relay (1.0)
vc	0.449	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.19	J/mol×K	454.97	Joback Method
cpg	275.17	J/mol×K	485.39	Joback Method
cpg	286.67	J/mol×K	515.81	Joback Method
cpg	297.72	J/mol×K	546.22	Joback Method
cpg	308.30	J/mol×K	576.64	Joback Method
cpg	318.44	J/mol×K	607.06	Joback Method
cpg	328.12	J/mol×K	637.48	Joback Method

dvisc	0.0043324	Pa×s	235.32	Joback Method
dvisc	0.0019397	Pa×s	271.93	Joback Method
dvisc	0.0010509	Pa×s	308.54	Joback Method
dvisc	0.0006484	Pa×s	345.14	Joback Method
dvisc	0.0004389	Pa×s	381.75	Joback Method
dvisc	0.0003181	Pa×s	418.36	Joback Method
dvisc	0.0002428	Pa×s	454.97	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45611e+01
Coeff. B	-3.79182e+03
Coeff. C	-6.15660e+01
Temperature range (K), min.	327.22
Temperature range (K), max.	471.51

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C44914036&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
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume