2-Propenoic acid, 2-methyl-, 2-methylpropyl ester

Other names: 2-Methylpropyl methacrylate
Blemmer IBMA
Isobutyl 2-methyl-2-propenoate
Isobutyl methacrylate
Isobutyl «alpha»-methacrylate
Isobutyl «alpha»-methylacrylate
Isobutyl Â«alphaÂ»-methacrylate
Isobutyl Â«alphaÂ»-methylacrylate
Isobutylester kyseliny methakrylove
Methacrylic acid, isobutyl ester
NSC 18607
UN 2283

Inchi: InChI=1S/C8H14O2/c1-6(2)5-10-8(9)7(3)4/h6H,3,5H2,1-2,4H3

InchiKey: RUMACXVDVNRZJZ-UHFFFAOYSA-N

Formula: C8H14O2

SMILES: C=C(C)C(=O)OCC(C)C

Mol. weight [g/mol]: 142.20

CAS: 97-86-9

Physical Properties

Property code	Value	Unit	Source
gf	-140.59	kJ/mol	Joback Method
hf	-342.89	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	41.58	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.762		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpol	928.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	923.00		NIST Webbook

rinpol	926.00		NIST Webbook
rinpol	926.00		NIST Webbook
ripol	1173.00		NIST Webbook
ripol	1162.00		NIST Webbook
ripol	1173.00		NIST Webbook
tb	428.20	K	NIST Webbook
tc	640.80	K	Joback Method
tf	221.36	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.11	J/mol×K	454.85	Joback Method
cpg	275.28	J/mol×K	485.84	Joback Method
cpg	286.96	J/mol×K	516.83	Joback Method
cpg	298.16	J/mol×K	547.83	Joback Method
cpg	308.88	J/mol×K	578.82	Joback Method
cpg	319.14	J/mol×K	609.81	Joback Method
cpg	328.94	J/mol×K	640.80	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53691e+01
Coeff. B	-3.95655e+03
Coeff. C	-6.01760e+01
Temperature range (K), min.	322.52
Temperature range (K), max.	453.56

Sources

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=C97869&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Liquid-Liquid Equilibria of Water + 2-Butanol + (Methyl Methacrylate or Butyl Methacrylate or Isobutyl Methacrylate) at (288.2 and 318.2) K:	https://www.doi.org/10.1021/je7002572
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Liquid liquid equilibria for the ternary systems water + 1-propanol + methyl methacrylate, + butyl methacrylate, and + isobutyl methacrylate:	https://www.doi.org/10.1016/j.fluid.2007.05.018
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Liquid liquid equilibria of water + 1-butanol + methyl methacrylate or butyl methacrylate or isobutyl methacrylate:	https://www.doi.org/10.1016/j.fluid.2007.07.011
Liquid-Liquid Equilibria for the Ternary Systems Water + 2-Propanol + Methyl Methacrylate at 288.15K and 318.15K: Methacrylate, + Butyl Methacrylate, and + Isobutyl Methacrylate:	https://www.doi.org/10.1021/je700118q

Legend

cpg:	Ideal gas heat capacity
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume