Isobutyl acrylate

Other names:	2-Methylpropyl acrylate
	2-Propenoic acid, 2-methylpropyl ester
	Acrylic acid, isobutyl ester
	Isobutyl 2-propenoate
	Isobutyl propenoate
	Isobutylester kyseliny akrylove
	NSC 20949
Inchi:	InChI=1S/C7H12O2/c1-4-7(8)9-5-6(2)3/h4,6H,1,5H2,2-3H3
InchiKey:	CFVWNXQPGQOHRJ-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	C=CC(=O)OCC(C)C
Mol. weight [g/mol]:	128.17
CAS:	106-63-8

Physical Properties

Property code	Value	Unit	Source
gf	-140.46	kJ/mol	Joback Method
hf	-312.46	kJ/mol	Joback Method
hfus	11.87	kJ/mol	Joback Method
hvap	39.27	kJ/mol	Joback Method
log10ws	-1.21		Aqueous Solubility Prediction Method
logp	1.372		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
rinpol	838.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	836.00		NIST Webbook
ripol	1109.00		NIST Webbook
ripol	1114.00		NIST Webbook
ripol	1107.00		NIST Webbook
ripol	1115.00		NIST Webbook
ripol	1107.00		NIST Webbook
ripol	1114.00		NIST Webbook
tb	405.00 ± 5.00	K	NIST Webbook

tb	405.20	K	NIST Webbook
tb	421.95	K	NIST Webbook
tc	616.21	K	Joback Method
tf	209.15	K	NIST Webbook
tf	212.10 ± 0.60	K	NIST Webbook
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.64	J/mol×K	616.21	Joback Method
cpg	272.85	J/mol×K	585.52	Joback Method
cpg	263.67	J/mol×K	554.84	Joback Method
cpg	254.10	J/mol×K	524.15	Joback Method
cpg	244.12	J/mol×K	493.46	Joback Method
cpg	233.73	J/mol×K	462.78	Joback Method
cpg	222.93	J/mol×K	432.09	Joback Method
dvisc	0.0042260	Pa×s	224.05	Joback Method
dvisc	0.0002529	Pa×s	432.09	Joback Method
dvisc	0.0003294	Pa×s	397.42	Joback Method
dvisc	0.0004515	Pa×s	362.74	Joback Method
dvisc	0.0006615	Pa×s	328.07	Joback Method
dvisc	0.0010605	Pa×s	293.40	Joback Method
dvisc	0.0019297	Pa×s	258.72	Joback Method
hvapt	43.80	kJ/mol	370.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.10065e+01
Coeff. B	-8.30899e+03
Coeff. C	-1.11903e+01
Coeff. D	7.50743e-06
Temperature range (K), min.	212.00
Temperature range (K), max.	580.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1182.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106638&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1182
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
hvapt:	Enthalpy of vaporization at a given temperature
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