Crotonic acid

Other names:	.alpha.-butenoic acid
	2-Butenoic acid
	2-butenoic acid (isomer not specified)
	3-Methylacrylic acid
	Acrylic acid, 3-methyl-
	But-2-enoic acid
	CH3CH=CHCOOH
	Kyselina krotonova
	NSC 206946
	UN 2823
	butenoic acid
	«alpha»-Butenoic acid
	«alpha»-Crotonic acid
	«beta»-Methylacrylic acid
	Â«alphaÂ»-Butenoic acid
	Â«alphaÂ»-Crotonic acid
	Â«betaÂ»-Methylacrylic acid
Inchi:	InChI=1S/C4H6O2/c1-2-3-4(5)6/h2-3H,1H3,(H,5,6)
InchiKey:	LDHQCZJRKDOVOX-UHFFFAOYSA-N
Formula:	C4H6O2
SMILES:	CC=CC(=O)O
Mol. weight [g/mol]:	86.09
CAS:	3724-65-0

Physical Properties

Property code	Value	Unit	Source
chs	-1990.80 ± 1.00	kJ/mol	NIST Webbook
chs	-1999.00	kJ/mol	NIST Webbook
gf	-202.72	kJ/mol	Joback Method
hf	-368.50 ± 1.40	kJ/mol	NIST Webbook
hfs	-440.70 ± 1.30	kJ/mol	NIST Webbook
hfus	12.01	kJ/mol	Joback Method
hsub	72.20 ± 0.40	kJ/mol	NIST Webbook
hsub	72.20	kJ/mol	NIST Webbook
hvap	47.88	kJ/mol	Joback Method
log10ws	9.52e-03		Aqueous Solubility Prediction Method

logp	0.647		Crippen Method
mcvol	70.360	ml/mol	McGowan Method
pc	5138.68	kPa	Joback Method
rinpol	986.00		NIST Webbook
ripol	1746.00		NIST Webbook
ripol	1708.00		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1763.00		NIST Webbook
ripol	1773.00		NIST Webbook
ripol	1708.00		NIST Webbook
ripol	1773.00		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1709.00		NIST Webbook
tb	441.13	K	Joback Method
tc	623.44	K	Joback Method
tf	239.40 ± 0.60	K	NIST Webbook
tf	345.00 ± 1.50	K	NIST Webbook
tf	341.00 ± 0.20	K	NIST Webbook
tf	344.80	K	Solubilities of crotonic acid in different organic solvents at severaltemperatures from (278.15 to 333.15) K
vc	0.265	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.47	J/mol×K	441.13	Joback Method
cpg	135.50	J/mol×K	471.51	Joback Method
cpg	141.22	J/mol×K	501.90	Joback Method
cpg	146.65	J/mol×K	532.28	Joback Method
cpg	151.79	J/mol×K	562.67	Joback Method
cpg	156.65	J/mol×K	593.05	Joback Method
cpg	161.26	J/mol×K	623.44	Joback Method
dvisc	0.0325411	Pa×s	240.51	Joback Method
dvisc	0.0085700	Pa×s	273.95	Joback Method
dvisc	0.0030171	Pa×s	307.38	Joback Method
dvisc	0.0013037	Pa×s	340.82	Joback Method
dvisc	0.0006544	Pa×s	374.26	Joback Method
dvisc	0.0003678	Pa×s	407.69	Joback Method
dvisc	0.0002256	Pa×s	441.13	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.77424e+01
Coeff. B	-4.90563e+03
Coeff. C	-6.90720e+01
Temperature range (K), min.	350.12
Temperature range (K), max.	486.29

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubilities of crotonic acid in different organic solvents at severaltemperatures from (278.15 to 333.15) K:	https://www.doi.org/10.1016/j.fluid.2013.06.038
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C3724650&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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

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