«beta»-Acetylacrylic acid

Other names:	4-Oxo-2-pentenoic acid
	Acetylacrylic acid
	3-Acetylacrylic acid
	2-Pentenoic acid, 4-oxo-
	4-Ketopentenoic acid
	«beta»-Acetoacrylic acid
	4-oxopent-2-en-2-oic acid
Inchi:	InChI=1S/C5H6O3/c1-4(6)2-3-5(7)8/h2-3H,1H3,(H,7,8)/b3-2+
InchiKey:	XGTKSWVCNVUVHG-NSCUHMNNSA-N
Formula:	C5H6O3
SMILES:	CC(=O)C=CC(=O)O
Mol. weight [g/mol]:	114.10
CAS:	4743-82-2

Physical Properties

Property code	Value	Unit	Source
gf	-323.22	kJ/mol	Joback Method
hf	-406.70	kJ/mol	Joback Method
hfus	16.19	kJ/mol	Joback Method
hvap	56.85	kJ/mol	Joback Method
log10ws	-0.15		Crippen Method
logp	0.216		Crippen Method
mcvol	86.020	ml/mol	McGowan Method
pc	4903.92	kPa	Joback Method
tb	517.88	K	Joback Method
tc	708.21	K	Joback Method
tf	301.71	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.08	J/mol×K	517.88	Joback Method
cpg	182.57	J/mol×K	549.60	Joback Method

cpg	188.70	J/mol×K	581.32	Joback Method
cpg	194.48	J/mol×K	613.05	Joback Method
cpg	199.93	J/mol×K	644.77	Joback Method
cpg	205.07	J/mol×K	676.49	Joback Method
cpg	209.90	J/mol×K	708.21	Joback Method
dvisc	0.0102256	Pa×s	301.71	Joback Method
dvisc	0.0035787	Pa×s	337.74	Joback Method
dvisc	0.0015334	Pa×s	373.77	Joback Method
dvisc	0.0007626	Pa×s	409.80	Joback Method
dvisc	0.0004246	Pa×s	445.82	Joback Method
dvisc	0.0002581	Pa×s	481.85	Joback Method
dvisc	0.0001681	Pa×s	517.88	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C4743822&Units=SI

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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume