4-methyl-2-pentenoic acid

Inchi: InChI=1S/C6H10O2/c1-5(2)3-4-6(7)8/h3-5H,1-2H3,(H,7,8)
InchiKey: QAOXMQCWUWZZNC-UHFFFAOYSA-N
Formula: C6H10O2
SMILES: CC(C)C=CC(=O)O
Mol. weight [g/mol]: 114.14
CAS: 10321-71-8

Physical Properties

Property code	Value	Unit	Source
hf	-430.96	kJ/mol	Cheméo Relay (1.0)
hfus	13.66	kJ/mol	Joback Method
hvap	65.43	kJ/mol	Cheméo Relay (1.0)
ie	9.82	eV	Cheméo Relay (1.0)
log10ws	-1.38		Cheméo Relay (1.0)
logp	1.283		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
tb	450.20	K	Cheméo Relay (1.0)
tc	623.54	K	Cheméo Relay (1.0)
tf	332.53	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.34	J/mol×K	486.45	Joback Method
cpg	252.21	J/mol×K	669.30	Joback Method
cpg	245.53	J/mol×K	638.82	Joback Method
cpg	238.49	J/mol×K	608.35	Joback Method
cpg	231.07	J/mol×K	577.87	Joback Method
cpg	223.25	J/mol×K	547.40	Joback Method
cpg	215.01	J/mol×K	516.92	Joback Method
dvisc	0.0010788	Pa×s	367.25	Joback Method
dvisc	0.0001605	Pa×s	486.45	Joback Method
dvisc	0.0002706	Pa×s	446.72	Joback Method

dvisc	0.0005050	Pa×s	406.98	Joback Method
dvisc	0.0452390	Pa×s	248.05	Joback Method
dvisc	0.0027706	Pa×s	327.52	Joback Method
dvisc	0.0092323	Pa×s	287.78	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57152e+01
Coeff. B	-4.57751e+03
Coeff. C	-7.74120e+01
Temperature range (K), min.	374.12
Temperature range (K), max.	517.40

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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):

Legend

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