2-Octenoic acid

Other names: Oct-2-enoic acid
Inchi: InChI=1S/C8H14O2/c1-2-3-4-5-6-7-8(9)10/h6-7H,2-5H2,1H3,(H,9,10)/b7-6+
InchiKey: CWMPPVPFLSZGCY-VOTSOKGWSA-N
Formula: C8H14O2
SMILES: CCCCCC=CC(=O)O
Mol. weight [g/mol]: 142.20
CAS: 1470-50-4

Physical Properties

Property code	Value	Unit	Source
gf	-169.04	kJ/mol	Joback Method
hf	-356.04	kJ/mol	Joback Method
hfus	22.36	kJ/mol	Joback Method
hvap	56.78	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	2.208		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
tb	518.15 ± 2.00	K	NIST Webbook
tc	708.47	K	Joback Method
tf	285.59	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.94	J/mol×K	532.65	Joback Method
cpg	301.30	J/mol×K	561.95	Joback Method
cpg	311.18	J/mol×K	591.26	Joback Method
cpg	320.59	J/mol×K	620.56	Joback Method
cpg	329.56	J/mol×K	649.86	Joback Method
cpg	338.09	J/mol×K	679.17	Joback Method
cpg	346.22	J/mol×K	708.47	Joback Method
dvisc	0.0161455	Pa×s	285.59	Joback Method

dvisc	0.0042862	Pa×s	326.77	Joback Method
dvisc	0.0015311	Pa×s	367.94	Joback Method
dvisc	0.0006729	Pa×s	409.12	Joback Method
dvisc	0.0003437	Pa×s	450.30	Joback Method
dvisc	0.0001965	Pa×s	491.47	Joback Method
dvisc	0.0001225	Pa×s	532.65	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41450e+01
Coeff. B	-4.25411e+03
Coeff. C	-8.28880e+01
Temperature range (K), min.	389.88
Temperature range (K), max.	564.47

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=C1470504&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume