2-Propenoic acid, hexyl ester

Other names:	2-Propenoic acid,n-hexyl ester
	Acrylic acid, hexyl ester
	Ageflex FA-6
	Ageflex N-HA
	Hexyl 2-propenoate
	Hexyl acrylate
	NSC 11786
Inchi:	InChI=1S/C9H16O2/c1-3-5-6-7-8-11-9(10)4-2/h4H,2-3,5-8H2,1H3
InchiKey:	LNMQRPPRQDGUDR-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	C=CC(=O)OCCCCCC
Mol. weight [g/mol]:	156.23
CAS:	2499-95-8

Physical Properties

Property code	Value	Unit	Source
af	0.5802		Cheméo Relay (1.0)
hf	-430.87	kJ/mol	Cheméo Relay (1.0)
hfus	20.57	kJ/mol	Joback Method
hvap	51.39	kJ/mol	Cheméo Relay (1.0)
ie	10.06	eV	Cheméo Relay (1.0)
log10ws	-2.87		Cheméo Relay (1.0)
logp	2.296		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	1075.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1075.00		NIST Webbook
ripol	1374.00		NIST Webbook
ripol	1388.00		NIST Webbook
ripol	1392.00		NIST Webbook
ripol	1362.00		NIST Webbook

ripol	1370.00		NIST Webbook
tb	452.85	K	Cheméo Relay (1.0)
tc	646.34	K	Cheméo Relay (1.0)
tf	221.09	K	Cheméo Relay (1.0)
vc	0.528	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.97	J/mol×K	625.83	Joback Method
cpg	374.26	J/mol×K	655.34	Joback Method
cpg	318.12	J/mol×K	507.80	Joback Method
cpg	330.31	J/mol×K	537.31	Joback Method
cpg	342.00	J/mol×K	566.81	Joback Method
cpg	353.22	J/mol×K	596.32	Joback Method
cpg	305.44	J/mol×K	478.29	Joback Method
dvisc	0.0009072	Pa×s	333.82	Joback Method
dvisc	0.0015428	Pa×s	297.71	Joback Method
dvisc	0.0030378	Pa×s	261.59	Joback Method
dvisc	0.0005918	Pa×s	369.94	Joback Method
dvisc	0.0004165	Pa×s	406.06	Joback Method
dvisc	0.0003104	Pa×s	442.17	Joback Method
dvisc	0.0002419	Pa×s	478.29	Joback Method
hvapt	48.20	kJ/mol	401.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58377e+01
Coeff. B	-4.40236e+03
Coeff. C	-7.12340e+01
Temperature range (K), min.	354.34
Temperature range (K), max.	489.46

Sources

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):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2499958&Units=SI

Legend

af:	Acentric Factor
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
hvapt:	Enthalpy of vaporization at a given temperature
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
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