2-Hexenal, 2-ethyl-

Other names:	2-Ethyl-2-hexen-1-al
	2-Ethyl-2-hexenal
	2-Ethyl-3-propylacrolein
	2-Ethylhexenal
	2-ethylhex-2-enal
	Acrolein, 2-ethyl-3-propyl-
	NSC 4787
	«alpha»-Ethyl-2-hexenal
	«alpha»-Ethyl-«beta»-n-propylacrolein
	«alpha»-Ethyl-«beta»-propylacrolein
	Â«alphaÂ»-Ethyl-2-hexenal
	Â«alphaÂ»-Ethyl-Â«betaÂ»-n-propylacrolein
	Â«alphaÂ»-Ethyl-Â«betaÂ»-propylacrolein
Inchi:	InChI=1S/C8H14O/c1-3-5-6-8(4-2)7-9/h6-7H,3-5H2,1-2H3/b8-6-
InchiKey:	PYLMCYQHBRSDND-VURMDHGXSA-N
Formula:	C8H14O
SMILES:	CCCC=C(C=O)CC
Mol. weight [g/mol]:	126.20
CAS:	645-62-5

Physical Properties

Property code	Value	Unit	Source
chl	-4887.62 ± 0.71	kJ/mol	NIST Webbook
gf	-11.37	kJ/mol	Joback Method
hf	-186.60	kJ/mol	Joback Method
hfl	-261.30 ± 0.71	kJ/mol	NIST Webbook
hfus	17.66	kJ/mol	Joback Method
hvap	40.16	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.322		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	968.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	964.00		NIST Webbook

rinpol	1007.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1011.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1336.00		NIST Webbook
tb	450.20 ± 0.30	K	NIST Webbook
tb	441.65 ± 2.00	K	NIST Webbook
tb	445.15 ± 2.00	K	NIST Webbook
tb	444.65 ± 3.00	K	NIST Webbook
tc	617.65	K	Joback Method
tf	202.88	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.01	J/mol×K	435.14	Joback Method
cpg	253.06	J/mol×K	465.56	Joback Method
cpg	264.55	J/mol×K	495.98	Joback Method
cpg	275.48	J/mol×K	526.39	Joback Method
cpg	285.90	J/mol×K	556.81	Joback Method
cpg	295.81	J/mol×K	587.23	Joback Method
cpg	305.24	J/mol×K	617.65	Joback Method
hvapt	48.40	kJ/mol	387.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	345.50 ± 1.50	K	4.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.48064e+01
Coeff. B	-3.91694e+03
Coeff. C	-6.57360e+01
Temperature range (K), min.	335.52
Temperature range (K), max.	478.27

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=C645625&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

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume