

2-Ethylacrolein

Other names:	1,4-Pentadiene-3-ol 2-Ethacrolein 2-Ethylpropenal 2-ethylacrylaldehyde Butanal, 2-methylene-
Inchi:	InChI=1S/C5H8O/c1-3-5(2)4-6/h4H,2-3H2,1H3
InchiKey:	GMLDCZYTIPCVMO-UHFFFAOYSA-N
Formula:	C5H8O
SMILES:	C=C(C=O)CC
Mol. weight [g/mol]:	84.12
CAS:	922-63-4

Physical Properties

Property code	Value	Unit	Source
chl	-2946.60 ± 2.50	kJ/mol	NIST Webbook
gf	-29.01	kJ/mol	Joback Method
hf	-131.20 ± 2.60	kJ/mol	NIST Webbook
hfl	-168.00 ± 2.60	kJ/mol	NIST Webbook
hfus	8.40	kJ/mol	Joback Method
hvap	36.80	kJ/mol	NIST Webbook
hvap	36.80 ± 0.40	kJ/mol	NIST Webbook
hvap	36.81 ± 0.41	kJ/mol	NIST Webbook
log10ws	-1.05		Crippen Method
logp	1.151		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
ripol	974.00		NIST Webbook
ripol	957.00		NIST Webbook
ripol	957.00		NIST Webbook
tb	365.70	K	NIST Webbook
tc	539.23	K	Joback Method
tf	172.39	K	Joback Method
vc	0.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	131.28	J/mol×K	359.02	Joback Method
cpg	139.14	J/mol×K	389.06	Joback Method
cpg	146.64	J/mol×K	419.09	Joback Method
cpg	153.82	J/mol×K	449.13	Joback Method
cpg	160.67	J/mol×K	479.16	Joback Method
cpg	167.22	J/mol×K	509.20	Joback Method
cpg	173.46	J/mol×K	539.23	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48269e+01
Coeff. B	-3.29634e+03
Coeff. C	-4.28010e+01
Temperature range (K), min.	269.52
Temperature range (K), max.	389.22

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=C922634&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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