2-Hexen-1-ol, 2-ethyl-

Other names: 2-Ethyl-2-hexen-1-ol
2-ethylhex-2-enol
Inchi: InChI=1S/C8H16O/c1-3-5-6-8(4-2)7-9/h6,9H,3-5,7H2,1-2H3/b8-6+
InchiKey: JSRFYJBJQPGAAA-SOFGYWHQSA-N
Formula: C8H16O
SMILES: CCCC=C(CC)CO
Mol. weight [g/mol]: 128.21
CAS: 50639-00-4

Physical Properties

Property code	Value	Unit	Source
gf	-48.67	kJ/mol	Joback Method
hf	-253.25	kJ/mol	Joback Method
hfus	19.46	kJ/mol	Joback Method
hvap	50.12	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.115		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
rinpol	989.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	1002.00		NIST Webbook
ripol	1518.00		NIST Webbook
tb	478.66	K	Joback Method
tc	648.23	K	Joback Method
tf	221.70	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.19	J/mol×K	478.66	Joback Method
cpg	284.54	J/mol×K	506.92	Joback Method

cpg	295.39	J/mol×K	535.18	Joback Method
cpg	305.77	J/mol×K	563.45	Joback Method
cpg	315.70	J/mol×K	591.71	Joback Method
cpg	325.18	J/mol×K	619.97	Joback Method
cpg	334.25	J/mol×K	648.23	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50639004&Units=SI

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

Legend

cpg: Ideal gas heat capacity
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
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