ETHANOL, 2-(PROPYLTHIO)-

Other names:	2-(propylthio)ethanol
	2-Hydroxyethyl n-propyl sulfide
	Ethanol, 2-(propylthio)-
	«beta»-Hydroxyethyl-n-propyl sulfide
Inchi:	InChI=1S/C5H12OS/c1-2-4-7-5-3-6/h6H,2-5H2,1H3
InchiKey:	KCWWXXYQPUDKBX-UHFFFAOYSA-N
Formula:	C5H12OS
SMILES:	CCCSCCO
Mol. weight [g/mol]:	120.22

Physical Properties

Property code	Value	Unit	Source
af	0.5964		Cheméo Relay (1.0)
gf	-112.48	kJ/mol	Joback Method
hf	-283.32	kJ/mol	Cheméo Relay (1.0)
hfus	16.92	kJ/mol	Joback Method
hvap	64.10	kJ/mol	Cheméo Relay (1.0)
ie	8.93	eV	Cheméo Relay (1.0)
log10ws	-0.39		Cheméo Relay (1.0)
logp	1.122		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	466.98	K	Cheméo Relay (1.0)
tc	691.62	K	Cheméo Relay (1.0)
tf	209.71	K	Cheméo Relay (1.0)
vc	0.357	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.57	J/mol×K	474.76	Joback Method
cpg	222.54	J/mol×K	505.12	Joback Method
cpg	231.16	J/mol×K	535.49	Joback Method
cpg	239.43	J/mol×K	565.85	Joback Method

cpg	247.36	J/mol×K	596.22	Joback Method
cpg	254.95	J/mol×K	626.58	Joback Method
cpg	262.20	J/mol×K	656.94	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22812904&Units=SI

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

Legend

af: Acentric Factor
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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume