2-(ISOPROPYLTHIO)ETHANOL

Other names: Ethanol, 2-[(1-methylethyl)thio]-
2-[(1-methylethyl)thio]ethanol
Inchi: InChI=1S/C5H12OS/c1-5(2)7-4-3-6/h5-6H,3-4H2,1-2H3
InchiKey: QGONIKZRWOOHBB-UHFFFAOYSA-N
Formula: C5H12OS
SMILES: CC(C)SCCO
Mol. weight [g/mol]: 120.22

Physical Properties

Property code	Value	Unit	Source
hf	-284.86	kJ/mol	Cheméo Relay (1.0)
hfus	13.40	kJ/mol	Joback Method
hvap	61.99	kJ/mol	Cheméo Relay (1.0)
ie	8.73	eV	Cheméo Relay (1.0)
logp	1.120		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
tb	456.75	K	Cheméo Relay (1.0)
tf	208.92	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.79	J/mol×K	474.32	Joback Method
cpg	223.03	J/mol×K	505.35	Joback Method
cpg	231.90	J/mol×K	536.37	Joback Method
cpg	240.40	J/mol×K	567.40	Joback Method
cpg	248.53	J/mol×K	598.42	Joback Method
cpg	256.30	J/mol×K	629.45	Joback Method
cpg	263.71	J/mol×K	660.48	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40811492&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
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point