Ethanol, 2-hexadecylthio-

Inchi: InChI=1S/C18H38OS/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-17-20-18-16-19/h19H,2-18H
InchiKey: PDOIABQTPMOHQQ-UHFFFAOYSA-N
Formula: C18H38OS
SMILES: CCCCCCCCCCCCCCCCSCCO
Mol. weight [g/mol]: 302.56
CAS: 23248-47-7

Physical Properties

Property code	Value	Unit	Source
gf	-3.02	kJ/mol	Joback Method
hf	-525.21	kJ/mol	Joback Method
hfus	50.59	kJ/mol	Joback Method
hvap	79.16	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	6.193		Crippen Method
mcvol	286.700	ml/mol	McGowan Method
pc	1242.46	kPa	Joback Method
tb	772.20	K	Joback Method
tc	949.73	K	Joback Method
tf	387.84	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.17	J/mol×K	772.20	Joback Method
cpg	895.87	J/mol×K	801.79	Joback Method
cpg	912.69	J/mol×K	831.38	Joback Method
cpg	928.66	J/mol×K	860.97	Joback Method
cpg	943.81	J/mol×K	890.55	Joback Method
cpg	958.17	J/mol×K	920.14	Joback Method
cpg	971.78	J/mol×K	949.73	Joback Method

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=C23248477&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume