2-Hydroxyethyl hexyl sulfide

Other names: 2-(hexylthio)ethanol
Inchi: InChI=1S/C8H18OS/c1-2-3-4-5-7-10-8-6-9/h9H,2-8H2,1H3
InchiKey: ZMGLDPZVDZFNLE-UHFFFAOYSA-N
Formula: C8H18OS
SMILES: CCCCCCSCCO
Mol. weight [g/mol]: 162.29
CAS: 24475-56-7

Physical Properties

Property code	Value	Unit	Source
gf	-87.22	kJ/mol	Joback Method
hf	-318.81	kJ/mol	Joback Method
hfus	24.69	kJ/mol	Joback Method
hvap	56.90	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.292		Crippen Method
mcvol	145.800	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
rinpol	1317.00		NIST Webbook
tb	543.40	K	Joback Method
tc	720.44	K	Joback Method
tf	275.14	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.03	J/mol×K	543.40	Joback Method
cpg	355.00	J/mol×K	572.91	Joback Method
cpg	366.48	J/mol×K	602.41	Joback Method
cpg	377.46	J/mol×K	631.92	Joback Method
cpg	387.96	J/mol×K	661.43	Joback Method
cpg	397.99	J/mol×K	690.94	Joback Method
cpg	407.56	J/mol×K	720.44	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=C24475567&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume