Disulfide, ethyl hexyl

Other names: Ethyl hexyl disulfide
Inchi: InChI=1S/C8H18S2/c1-3-5-6-7-8-10-9-4-2/h3-8H2,1-2H3
InchiKey: YKNTWULGFXMYRB-UHFFFAOYSA-N
Formula: C8H18S2
SMILES: CCCCCCSSCC
Mol. weight [g/mol]: 178.36

Physical Properties

Property code	Value	Unit	Source
gf	82.72	kJ/mol	Joback Method
hf	-124.71	kJ/mol	Joback Method
hfus	24.74	kJ/mol	Joback Method
hvap	47.04	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.968		Crippen Method
mcvol	156.280	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
ripol	1596.00		NIST Webbook
tb	520.00	K	Joback Method
tc	726.00	K	Joback Method
tf	248.72	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.73	J/mol×K	520.00	Joback Method
cpg	355.21	J/mol×K	554.33	Joback Method
cpg	369.03	J/mol×K	588.67	Joback Method
cpg	382.19	J/mol×K	623.00	Joback Method
cpg	394.70	J/mol×K	657.33	Joback Method
cpg	406.56	J/mol×K	691.67	Joback Method
cpg	417.78	J/mol×K	726.00	Joback Method

Sources

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=U75512&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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