2-[Hexylthio]ethanal

Inchi: InChI=1S/C8H16OS/c1-2-3-4-5-7-10-8-6-9/h6H,2-5,7-8H2,1H3
InchiKey: FWYYDAZHINHUBD-UHFFFAOYSA-N
Formula: C8H16OS
SMILES: CCCCCCSCC=O
Mol. weight [g/mol]: 160.28

Physical Properties

Property code	Value	Unit	Source
gf	-49.92	kJ/mol	Joback Method
hf	-252.16	kJ/mol	Joback Method
hfus	22.89	kJ/mol	Joback Method
hvap	46.94	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.499		Crippen Method
mcvol	141.500	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
ripol	1745.00		NIST Webbook
ripol	1745.00		NIST Webbook
tb	499.88	K	Joback Method
tc	690.77	K	Joback Method
tf	256.32	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.66	J/mol×K	499.88	Joback Method
cpg	321.40	J/mol×K	531.69	Joback Method
cpg	333.57	J/mol×K	563.51	Joback Method
cpg	345.20	J/mol×K	595.32	Joback Method
cpg	356.28	J/mol×K	627.14	Joback Method
cpg	366.83	J/mol×K	658.95	Joback Method
cpg	376.86	J/mol×K	690.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R402125&Units=SI
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

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