3-Sulfanylhexanal

Inchi: InChI=1S/C6H12OS/c1-2-3-6(8)4-5-7/h5-6,8H,2-4H2,1H3
InchiKey: MMODARXIJRCRGL-UHFFFAOYSA-N
Formula: C6H12OS
SMILES: CCCC(S)CC=O
Mol. weight [g/mol]: 132.22

Physical Properties

Property code	Value	Unit	Source
gf	-72.93	kJ/mol	Joback Method
hf	-219.55	kJ/mol	Joback Method
hfus	14.10	kJ/mol	Joback Method
hvap	42.02	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.674		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
rinpol	1013.00		NIST Webbook
ripol	1544.00		NIST Webbook
tb	447.76	K	Joback Method
tc	647.73	K	Joback Method
tf	220.84	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.70	J/mol×K	447.76	Joback Method
cpg	234.50	J/mol×K	481.09	Joback Method
cpg	244.79	J/mol×K	514.42	Joback Method
cpg	254.59	J/mol×K	547.74	Joback Method
cpg	263.90	J/mol×K	581.07	Joback Method
cpg	272.74	J/mol×K	614.40	Joback Method
cpg	281.12	J/mol×K	647.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R621386&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume