3-Sulfanylheptanal

Inchi: InChI=1S/C7H14OS/c1-2-3-4-7(9)5-6-8/h6-7,9H,2-5H2,1H3
InchiKey: IIEVDYNDUAHALL-UHFFFAOYSA-N
Formula: C7H14OS
SMILES: CCCCC(S)CC=O
Mol. weight [g/mol]: 146.25

Physical Properties

Property code	Value	Unit	Source
gf	-64.51	kJ/mol	Joback Method
hf	-240.19	kJ/mol	Joback Method
hfus	16.69	kJ/mol	Joback Method
hvap	44.25	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.064		Crippen Method
mcvol	127.410	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
rinpol	1113.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1118.00		NIST Webbook
ripol	1665.00		NIST Webbook
ripol	1659.00		NIST Webbook
ripol	1659.00		NIST Webbook
tb	470.64	K	Joback Method
tc	668.23	K	Joback Method
tf	232.11	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.16	J/mol×K	470.64	Joback Method
cpg	276.15	J/mol×K	503.57	Joback Method
cpg	287.57	J/mol×K	536.50	Joback Method
cpg	298.44	J/mol×K	569.43	Joback Method

cpg	308.78	J/mol×K	602.36	Joback Method
cpg	318.59	J/mol×K	635.29	Joback Method
cpg	327.90	J/mol×K	668.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R609915&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