3-sulfanylheptanal

Inchi: InChI=1S/C8H16OS/c1-3-4-5-8(10-2)6-7-9/h7-8H,3-6H2,1-2H3
InchiKey: RQOSXGWCILNIKB-UHFFFAOYSA-N
Formula: C8H16OS
SMILES: CCCCC(CC=O)SC
Mol. weight [g/mol]: 160.28

Physical Properties

Property code	Value	Unit	Source
gf	-52.36	kJ/mol	Joback Method
hf	-257.44	kJ/mol	Joback Method
hfus	19.37	kJ/mol	Joback Method
hvap	46.55	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.497		Crippen Method
mcvol	141.500	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
rinpol	1118.00		NIST Webbook
ripol	1659.00		NIST Webbook
ripol	1659.00		NIST Webbook
tb	499.44	K	Joback Method
tc	694.49	K	Joback Method
tf	241.32	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.89	J/mol×K	499.44	Joback Method
cpg	321.98	J/mol×K	531.95	Joback Method
cpg	334.48	J/mol×K	564.46	Joback Method
cpg	346.39	J/mol×K	596.96	Joback Method
cpg	357.72	J/mol×K	629.47	Joback Method
cpg	368.50	J/mol×K	661.98	Joback Method
cpg	378.72	J/mol×K	694.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R419782&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

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