3-Mercaptooctanal

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

Physical Properties

Property code	Value	Unit	Source
gf	-56.09	kJ/mol	Joback Method
hf	-260.83	kJ/mol	Joback Method
hfus	19.28	kJ/mol	Joback Method
hvap	46.47	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.454		Crippen Method
mcvol	141.500	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	1268.00		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1214.00		NIST Webbook
tb	493.52	K	Joback Method
tc	688.66	K	Joback Method
tf	243.38	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.71	J/mol×K	493.52	Joback Method
cpg	319.75	J/mol×K	526.04	Joback Method
cpg	332.17	J/mol×K	558.57	Joback Method
cpg	343.99	J/mol×K	591.09	Joback Method
cpg	355.23	J/mol×K	623.62	Joback Method
cpg	365.90	J/mol×K	656.14	Joback Method
cpg	376.03	J/mol×K	688.66	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=R205553&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume