Octyl thioglycolate

Other names: Acetic acid, mercapto-, octyl ester
octyl mercaptoacetate
Inchi: InChI=1S/C10H20O2S/c1-2-3-4-5-6-7-8-12-10(11)9-13/h13H,2-9H2,1H3
InchiKey: MADOXCFISYCULS-UHFFFAOYSA-N
Formula: C10H20O2S
SMILES: CCCCCCCCOC(=O)CS
Mol. weight [g/mol]: 204.33
CAS: 7664-80-4

Physical Properties

Property code	Value	Unit	Source
gf	-171.21	kJ/mol	Joback Method
hf	-456.05	kJ/mol	Joback Method
hfus	28.48	kJ/mol	Joback Method
hvap	53.75	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.820		Crippen Method
mcvol	175.550	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
tb	567.35	K	Joback Method
tc	756.90	K	Joback Method
tf	311.08	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.59	J/mol×K	567.35	Joback Method
cpg	437.09	J/mol×K	598.94	Joback Method
cpg	450.94	J/mol×K	630.53	Joback Method
cpg	464.15	J/mol×K	662.13	Joback Method
cpg	476.74	J/mol×K	693.72	Joback Method
cpg	488.71	J/mol×K	725.31	Joback Method
cpg	500.07	J/mol×K	756.90	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7664804&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume