Isooctyl thioglycolate

Other names:	Isooctyl thioglycolate
	Acetic acid, mercapto-, isooctyl ester
Inchi:	InChI=1S/C10H20O2S/c1-9(2)6-4-3-5-7-12-10(11)8-13/h9,13H,3-8H2,1-2H3
InchiKey:	RZBBHEJLECUBJT-UHFFFAOYSA-N
Formula:	C10H20O2S
SMILES:	CC(C)CCCCCOC(=O)CS
Mol. weight [g/mol]:	204.34

Physical Properties

Property code	Value	Unit	Source
hf	-563.84	kJ/mol	Cheméo Relay (1.0)
hfus	24.96	kJ/mol	Joback Method
hvap	63.81	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.30		Cheméo Relay (1.0)
logp	2.676		Crippen Method
mcvol	175.550	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
tb	523.89	K	Cheméo Relay (1.0)
tc	716.92	K	Cheméo Relay (1.0)
tf	240.05	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.94	J/mol×K	566.91	Joback Method
cpg	437.78	J/mol×K	599.13	Joback Method
cpg	451.94	J/mol×K	631.34	Joback Method
cpg	465.43	J/mol×K	663.56	Joback Method
cpg	478.26	J/mol×K	695.77	Joback Method
cpg	490.44	J/mol×K	727.99	Joback Method
cpg	501.97	J/mol×K	760.21	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25103097&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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