

Isooctyl mercaptoacetate

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]:	204.33
CAS:	25103-09-7

Physical Properties

Property code	Value	Unit	Source
gf	-173.65	kJ/mol	Joback Method
hf	-461.33	kJ/mol	Joback Method
hfus	24.96	kJ/mol	Joback Method
hvap	53.36	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.676		Crippen Method
mvol	175.550	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
tb	566.91	K	Joback Method
tc	760.21	K	Joback Method
tf	296.08	K	Joback Method
vc	0.667	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25103097&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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