2-Octen-4-one, 5,5,6,6,7,7,8,8-octafluoro-2-mercapto-

Inchi: InChI=1S/C8H6F8OS/c1-3(18)2-4(17)6(11,12)8(15,16)7(13,14)5(9)10/h2,5,18H,1H3/b3-2

InchiKey: VHMCYEKUYBMISA-IHWYPQMZSA-N

Formula: C8H6F8OS

SMILES: CC(S)=CC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 302.19

CAS: 88552-04-9

Physical Properties

Property code	Value	Unit	Source
gf	-1563.78	kJ/mol	Joback Method
hf	-1775.53	kJ/mol	Joback Method
hfus	19.88	kJ/mol	Joback Method
hvap	36.11	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.560		Crippen Method
mcvol	151.360	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
tb	487.24	K	Joback Method
tc	658.56	K	Joback Method
tf	244.25	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.73	J/mol×K	487.24	Joback Method
cpg	375.16	J/mol×K	515.79	Joback Method
cpg	385.70	J/mol×K	544.35	Joback Method
cpg	395.40	J/mol×K	572.90	Joback Method
cpg	404.32	J/mol×K	601.45	Joback Method
cpg	412.50	J/mol×K	630.01	Joback Method
cpg	420.01	J/mol×K	658.56	Joback Method

Sources

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=C88552049&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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