4-Hexen-3-one, 1,1,2,2-tetrafluoro-5-mercapto-

Inchi: InChI=1S/C6H6F4OS/c1-3(12)2-4(11)6(9,10)5(7)8/h2,5,12H,1H3/b3-2-
InchiKey: JOMAVZMNUWTMSS-IHWYPQMZSA-N
Formula: C6H6F4OS
SMILES: CC(S)=CC(=O)C(F)(F)C(F)F
Mol. weight [g/mol]: 202.17
CAS: 64249-76-9

Physical Properties

Property code	Value	Unit	Source
gf	-807.06	kJ/mol	Joback Method
hf	-932.31	kJ/mol	Joback Method
hfus	17.21	kJ/mol	Joback Method
hvap	37.52	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.290		Crippen Method
mcvol	116.100	ml/mol	McGowan Method
pc	3217.33	kPa	Joback Method
tb	450.86	K	Joback Method
tc	640.02	K	Joback Method
tf	214.51	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.68	J/mol×K	450.86	Joback Method
cpg	251.51	J/mol×K	482.39	Joback Method
cpg	260.65	J/mol×K	513.91	Joback Method
cpg	269.15	J/mol×K	545.44	Joback Method
cpg	277.04	J/mol×K	576.97	Joback Method
cpg	284.36	J/mol×K	608.49	Joback Method
cpg	291.14	J/mol×K	640.02	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=C64249769&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume