4-Hepten-3-one, 1,1,2,2-tetrafluoro-5-mercapto-6,6-dimethyl-

Inchi: InChI=1S/C9H12F4OS/c1-8(2,3)6(15)4-5(14)9(12,13)7(10)11/h4,7,15H,1-3H3/b6-4-

InchiKey: PIVMKXHEJJWTBR-XQRVVYSFSA-N

Formula: C9H12F4OS

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

Mol. weight [g/mol]: 244.25

CAS: 64249-78-1

Physical Properties

Property code	Value	Unit	Source
gf	-778.96	kJ/mol	Joback Method
hf	-1002.98	kJ/mol	Joback Method
hfus	17.57	kJ/mol	Joback Method
hvap	42.90	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.316		Crippen Method
mcvol	158.370	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
tb	516.27	K	Joback Method
tc	710.50	K	Joback Method
tf	250.74	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.73	J/mol×K	516.27	Joback Method
cpg	385.12	J/mol×K	548.64	Joback Method
cpg	397.53	J/mol×K	581.01	Joback Method
cpg	409.04	J/mol×K	613.39	Joback Method
cpg	419.70	J/mol×K	645.76	Joback Method
cpg	429.59	J/mol×K	678.13	Joback Method
cpg	438.76	J/mol×K	710.50	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=C64249781&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