

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

Inchi:	InChI=1S/C9H12F4OS/c1-2-3-4-6(15)5-7(14)9(12,13)8(10)11/h5,8,15H,2-4H2,1H3/b6-5-
InchiKey:	MNHDCVLGHNJPRI-WAYWQWQTSA-N
Formula:	C9H12F4OS
SMILES:	CCCCC(S)=CC(=O)C(F)(F)C(F)F
Mol. weight [g/mol]:	244.25
CAS:	64249-77-0

Physical Properties

Property code	Value	Unit	Source
gf	-781.80	kJ/mol	Joback Method
hf	-994.23	kJ/mol	Joback Method
hfus	24.98	kJ/mol	Joback Method
hvap	44.20	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.460		Crippen Method
mcvol	158.370	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
tb	519.50	K	Joback Method
tc	702.74	K	Joback Method
tf	248.32	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.50	J/molxK	519.50	Joback Method
cpg	380.94	J/molxK	550.04	Joback Method
cpg	392.62	J/molxK	580.58	Joback Method
cpg	403.58	J/molxK	611.12	Joback Method
cpg	413.87	J/molxK	641.66	Joback Method
cpg	423.51	J/molxK	672.20	Joback Method
cpg	432.55	J/molxK	702.74	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=C64249770&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

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