1-Penten-3-one, 4,4,5,5-tetrafluoro-1-mercapto-1-phenyl-

Inchi: InChI=1S/C11H8F4OS/c12-10(13)11(14,15)9(16)6-8(17)7-4-2-1-3-5-7/h1-6,10,17H/b8-6-

InchiKey: MSLYGLCPYFMEDK-VURMDHGXSA-N

Formula: C11H8F4OS

SMILES: O=C(C=C(S)c1ccccc1)C(F)(F)C(F)F

Mol. weight [g/mol]: 264.24

CAS: 64249-79-2

Physical Properties

Property code	Value	Unit	Source
gf	-652.55	kJ/mol	Joback Method
hf	-798.98	kJ/mol	Joback Method
hfus	24.20	kJ/mol	Joback Method
hvap	50.92	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.427		Crippen Method
mcvol	162.790	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
tb	591.94	K	Joback Method
tc	810.47	K	Joback Method
tf	297.28	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.98	J/mol×K	591.94	Joback Method
cpg	400.50	J/mol×K	628.36	Joback Method
cpg	411.96	J/mol×K	664.78	Joback Method
cpg	422.44	J/mol×K	701.20	Joback Method
cpg	432.02	J/mol×K	737.62	Joback Method
cpg	440.80	J/mol×K	774.04	Joback Method
cpg	448.84	J/mol×K	810.47	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=C64249792&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