3-Octene-2-thione,5,5,6,6,7,7,8,8-octafluoro-4-hyd

Inchi: InChI=1S/C8H6F8OS/c1-3(18)2-4(17)6(11,12)8(15,16)7(13,14)5(9)10/h2,5,17H,1H3/b4-2

InchiKey: UUMGMYRXMQZTQL-RQOWECAXSA-N

Formula: C8H6F8OS

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

Mol. weight [g/mol]: 302.19

CAS: 88566-61-4

Physical Properties

Property code	Value	Unit	Source
gf	-1484.01	kJ/mol	Joback Method
hf	-1707.16	kJ/mol	Joback Method
hfus	22.93	kJ/mol	Joback Method
hvap	46.04	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.989		Crippen Method
mcvol	151.360	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
tb	532.73	K	Joback Method
tc	693.61	K	Joback Method
tf	252.95	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.19	J/mol×K	532.73	Joback Method
cpg	392.35	J/mol×K	559.54	Joback Method
cpg	400.74	J/mol×K	586.36	Joback Method
cpg	408.42	J/mol×K	613.17	Joback Method
cpg	415.45	J/mol×K	639.98	Joback Method
cpg	421.89	J/mol×K	666.80	Joback Method
cpg	427.80	J/mol×K	693.61	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=C88566614&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