

4-Heptene-3-thione,6,6,7,7-tetrafluoro-5-hydroxy-

Inchi:	InChI=1S/C7H8F4OS/c1-2-4(13)3-5(12)7(10,11)6(8)9/h3,6,12H,2H2,1H3/b5-3-
InchiKey:	ONTWAOHITSSBHD-HYXAFXHYSA-N
Formula:	C7H8F4OS
SMILES:	CCC(=S)C=C(O)C(F)(F)C(F)F
Mol. weight [g/mol]:	216.20
CAS:	88566-62-5

Physical Properties

Property code	Value	Unit	Source
gf	-718.87	kJ/mol	Joback Method
hf	-884.58	kJ/mol	Joback Method
hfus	22.85	kJ/mol	Joback Method
hvap	49.67	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.109		Crippen Method
mcvol	130.190	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
tb	519.23	K	Joback Method
tc	692.90	K	Joback Method
tf	234.48	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.35	J/molxK	519.23	Joback Method
cpg	308.16	J/molxK	548.17	Joback Method
cpg	316.33	J/molxK	577.12	Joback Method
cpg	323.91	J/molxK	606.06	Joback Method
cpg	330.95	J/molxK	635.01	Joback Method
cpg	337.50	J/molxK	663.95	Joback Method
cpg	343.61	J/molxK	692.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C88566625&Units=SI

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
mccvol:	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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