

4-Heptene-3-thione,6,6,7,7-tetrafluoro-5-hydroxy-2

Inchi:	InChI=1S/C8H10F4OS/c1-4(2)5(14)3-6(13)8(11,12)7(9)10/h3-4,7,13H,1-2H3/b6-3-
InchiKey:	QVFZBPQSLIKSIW-UTCJRWHEA-N
Formula:	C8H10F4OS
SMILES:	CC(C)C(=S)C=C(O)C(F)(F)C(F)F
Mol. weight [g/mol]:	230.22
CAS:	88552-01-6

Physical Properties

Property code	Value	Unit	Source
gf	-712.89	kJ/mol	Joback Method
hf	-910.50	kJ/mol	Joback Method
hfus	21.92	kJ/mol	Joback Method
hvap	51.51	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.355		Crippen Method
mcvol	144.280	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
tb	541.67	K	Joback Method
tc	717.20	K	Joback Method
tf	230.75	K	Joback Method
vc	0.569	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.22	J/molxK	541.67	Joback Method
cpg	353.00	J/molxK	570.93	Joback Method
cpg	362.11	J/molxK	600.18	Joback Method
cpg	370.59	J/molxK	629.44	Joback Method
cpg	378.50	J/molxK	658.69	Joback Method
cpg	385.88	J/molxK	687.95	Joback Method
cpg	392.79	J/molxK	717.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88552016&Units=SI
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

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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