3-Pentene-2-thione,5,5,5-trifluoro-4-hydroxy-

Inchi: InChI=1S/C5H5F3OS/c1-3(10)2-4(9)5(6,7)8/h2,9H,1H3/b4-2-
InchiKey: FQAMDKVTRBLKOJ-RQOWECAXSA-N
Formula: C5H5F3OS
SMILES: CC(=S)C=C(O)C(F)(F)F
Mol. weight [g/mol]: 170.15
CAS: 88551-99-9

Physical Properties

Property code	Value	Unit	Source
gf	-538.46	kJ/mol	Joback Method
hf	-641.91	kJ/mol	Joback Method
hfus	18.12	kJ/mol	Joback Method
hvap	46.42	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.380		Crippen Method
mcvol	100.240	ml/mol	McGowan Method
pc	4041.50	kPa	Joback Method
tb	474.64	K	Joback Method
tc	656.39	K	Joback Method
tf	226.35	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.08	J/mol×K	474.64	Joback Method
cpg	216.29	J/mol×K	504.93	Joback Method
cpg	222.89	J/mol×K	535.22	Joback Method
cpg	228.91	J/mol×K	565.51	Joback Method
cpg	234.42	J/mol×K	595.81	Joback Method
cpg	239.45	J/mol×K	626.10	Joback Method
cpg	244.06	J/mol×K	656.39	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C88551999&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume