

2-Butanone, 3-methylthio, PFBO # 2

Inchi: InChI=1S/C12H12F5NOS/c1-5(6(2)20-3)18-19-4-7-8(13)10(15)12(17)11(16)9(7)14/h6H,4
InchiKey: IBRSSDPLIBYCFA-UHFFFAOYSA-N
Formula: C12H12F5NOS
SMILES: CSC(C)C(C)=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 313.29

Physical Properties

Property code	Value	Unit	Source
hf	-1115.58	kJ/mol	Joback Method
hvap	56.04	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.026		Crippen Method
mcvol	192.930	ml/mol	McGowan Method
pc	1692.12	kPa	Joback Method
rinpol	1400.00		NIST Webbook
tb	689.21	K	Joback Method
tc	886.19	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R574666&Units=SI>
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

Legend

hf: Enthalpy of formation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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