

Butanal, 3-methylthio, PFBO # 1

Inchi: InChI=1S/C12H12F5NOS/c1-6(20-2)3-4-18-19-5-7-8(13)10(15)12(17)11(16)9(7)14/h4,6H
InchiKey: ZLJBOOAEGUCAMJ-UHFFFAOYSA-N
Formula: C12H12F5NOS
SMILES: CSC(C)CC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 313.29

Physical Properties

Property code	Value	Unit	Source
hf	-1105.79	kJ/mol	Joback Method
hvap	55.96	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.026		Crippen Method
mcvol	192.930	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
rinpol	1619.00		NIST Webbook
rinpol	1619.00		NIST Webbook
ripol	2139.00		NIST Webbook
tb	689.33	K	Joback Method
tc	883.69	K	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=R575283&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
r_{ipol}:	Polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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