

1,3-Butanedione, 4,4,4-trifluoro-1-(2-thienyl)-

Other names:	1,1,1-Trifluoro-3-(2-thienyl)acetone 1-(2-Thienyl)-3,3,3-trifluoroacetone 1-(Thienyl-(2'))-3,3,3-trifluoroacetone 1-Thienyl-3,3,3-trifluoroacetone 2-Thienyltrifluoroacetone 4,4,4-Trifluoro-1-(2-thienyl)-1,3-butanedione 4,4,4-trifluoro-1-(2-thienyl)butane-1,3-dione NSC 66544 TTA TTB Thienyltrifluoroacetone «alpha»-Thienyltrifluoroacetone Â«alphaÂ»-Thienyltrifluoroacetone
Inchi:	InChI=1S/C8H5F3O2S/c9-8(10,11)7(13)4-5(12)6-2-1-3-14-6/h1-3H,4H2
InchiKey:	TXBBUSUXYMIVOS-UHFFFAOYSA-N
Formula:	C8H5F3O2S
SMILES:	O=C(CC(=O)C(F)(F)F)c1cccs1
Mol. weight [g/mol]:	222.18
CAS:	326-91-0

Physical Properties

Property code	Value	Unit	Source
hsub	86.18 ± 0.64	kJ/mol	NIST Webbook
log10ws	-2.67		Crippen Method
logp	2.452		Crippen Method
mvol	128.920	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	370.20	K	1.00	NIST Webbook
tbrp	377.00	K	0.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.94282e+01
Coeff. B	-1.04459e+04
Temperature range (K), min.	358.47
Temperature range (K), max.	433.14

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C326910&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tbrp:	Boiling point at reduced pressure

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