Methanone, phenyl-2-thienyl-

Other names:	Ketone, phenyl 2-thienyl
	«alpha»-Benzoylthiophene
	Phenyl 2-thienyl ketone
	2-Benzoylthiophene
	2-Thienyl phenyl ketone
Inchi:	InChI=1S/C11H8OS/c12-11(10-7-4-8-13-10)9-5-2-1-3-6-9/h1-8H
InchiKey:	DWYFUJJWTRPARQ-UHFFFAOYSA-N
Formula:	C11H8OS
SMILES:	O=C(c1ccccc1)c1cccs1
Mol. weight [g/mol]:	188.25
CAS:	135-00-2

Physical Properties

Property code	Value	Unit	Source
ie	9.20 ± 0.10	eV	NIST Webbook
log10ws	-3.19		Crippen Method
logp	2.979		Crippen Method
mcvol	140.550	ml/mol	McGowan Method
tb	573.20	K	NIST Webbook
tb	573.00	K	NIST Webbook
tf	329.80 ± 0.20	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	414.50 ± 0.50	K	0.40	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C135002&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point