Thiophene, 2-ethyl-5-methyl-

Other names: 2-Methyl-5-ethyl-thiophene
2-Ethyl-5-methylthiophene
Inchi: InChI=1S/C7H10S/c1-3-7-5-4-6(2)8-7/h4-5H,3H2,1-2H3
InchiKey: VOIVNYVBGCJFRW-UHFFFAOYSA-N
Formula: C7H10S
SMILES: CCc1ccc(C)s1
Mol. weight [g/mol]: 126.22
CAS: 40323-88-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.51		Crippen Method
logp	2.619		Crippen Method
mcvol	106.380	ml/mol	McGowan Method
rinpol	967.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	945.00		NIST Webbook
tb	433.30 ± 2.00	K	NIST Webbook
tb	433.20 ± 1.50	K	NIST Webbook
tb	433.30 ± 1.50	K	NIST Webbook
tf	199.00 ± 1.00	K	NIST Webbook
tf	203.80 ± 1.50	K	NIST Webbook
tf	204.70 ± 0.80	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40323884&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point