2-BROMO-3-METHYLTHIOPHENE

Other names: 2-Bromo-3-methylthiophene
Inchi: InChI=1S/C5H5BrS/c1-4-2-3-7-5(4)6/h2-3H,1H3
InchiKey: YYJBWYBULYUKMR-UHFFFAOYSA-N
Formula: C5H5BrS
SMILES: Cc1ccsc1Br
Mol. weight [g/mol]: 177.07

Physical Properties

Property code	Value	Unit	Source
hvap	44.45	kJ/mol	Cheméo Relay (1.0)
logp	2.819		Crippen Method
mcvol	95.700	ml/mol	McGowan Method
tb	443.99	K	Cheméo Relay (1.0)
tf	235.61	K	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	300.20	K	0.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14282769&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

hvap:	Enthalpy of vaporization at standard conditions
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