

4-Nonylbenzo[b]thiophene

Other names:	4-Nonylbenzo[b]thiophene
Inchi:	InChI=1S/C17H24S/c1-2-3-4-5-6-7-8-10-15-11-9-12-17-16(15)13-14-18-17/h9,11-14H,2-
InchiKey:	BRFXDRPYWVUZKV-UHFFFAOYSA-N
Formula:	C17H24S
SMILES:	CCCCCCCCCc1cccc2sccc12
Mol. weight [g/mol]:	260.45

Physical Properties

Property code	Value	Unit	Source
af	0.7015		Cheméo Relay (1.0)
hvap	91.99	kJ/mol	Cheméo Relay (1.0)
ie	8.11	eV	Cheméo Relay (1.0)
logp	6.194		Crippen Method
mcvol	227.820	ml/mol	McGowan Method
pc	1847.31	kPa	Cheméo Relay (1.0, beta)
rinpol	2089.00		NIST Webbook
rinpol	2089.00		NIST Webbook
tb	634.37	K	Cheméo Relay (1.0)
tc	830.28	K	Cheméo Relay (1.0)
tf	296.98	K	Cheméo Relay (1.0)
vc	0.868	m3/kmol	Cheméo Relay (1.0)

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R41641&Units=SI

Legend

af:	Acentric Factor
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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