2-hexadecylthiophene

Inchi: InChI=1S/C20H36S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-17-20-18-16-19-21-20/h16,18
InchiKey: PJBTZAOJLKQEES-UHFFFAOYSA-N
Formula: C20H36S
SMILES: CCCCCCCCCCCCCCCCc1cccs1
Mol. weight [g/mol]: 308.56
CAS: 83027-72-9

Physical Properties

Property code	Value	Unit	Source
af	0.8514		Cheméo Relay (1.0)
hvap	103.13	kJ/mol	Cheméo Relay (1.0)
ie	8.87	eV	Cheméo Relay (1.0)
log10ws	-7.97		Cheméo Relay (1.0)
logp	7.772		Crippen Method
mcvol	289.550	ml/mol	McGowan Method
pc	1261.87	kPa	Cheméo Relay (1.0, beta)
tb	613.46	K	Cheméo Relay (1.0)
tc	798.85	K	Cheméo Relay (1.0)
tf	305.60	K	Cheméo Relay (1.0)
vc	1.132	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43800e+01
Coeff. B	-5.16259e+03
Coeff. C	-1.18222e+02
Temperature range (K), min.	484.56
Temperature range (K), max.	687.51

Sources

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):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C83027729&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume