

ANTHRACENE, 9,10-DIMETHOXY-

Inchi:	InChI=1S/C16H14O2/c1-17-15-11-7-3-5-9-13(11)16(18-2)14-10-6-4-8-12(14)15/h3-10H,1
InchiKey:	JWJMBKSFTTXMLL-UHFFFAOYSA-N
Formula:	C16H14O2
SMILES:	COc1c2ccccc2c(OC)c2ccccc12
Mol. weight [g/mol]:	238.29

Physical Properties

Property code	Value	Unit	Source
af	0.6213		Cheméo Relay (1.0)
hf	-71.14	kJ/mol	Cheméo Relay (1.0)
hfus	26.48	kJ/mol	Joback Method
hvap	100.16	kJ/mol	Cheméo Relay (1.0)
ie	7.56	eV	Cheméo Relay (1.0)
log10ws	-4.89		Cheméo Relay (1.0)
logp	4.010		Crippen Method
mcvol	185.360	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
tb	657.76	K	Cheméo Relay (1.0)
tc	929.46	K	Cheméo Relay (1.0)
tf	400.34	K	Cheméo Relay (1.0)
vc	0.686	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.26	J/mol×K	689.90	Joback Method
cpg	495.08	J/mol×K	729.41	Joback Method
cpg	508.88	J/mol×K	768.91	Joback Method
cpg	521.71	J/mol×K	808.42	Joback Method
cpg	533.66	J/mol×K	847.92	Joback Method
cpg	544.79	J/mol×K	887.43	Joback Method
cpg	555.15	J/mol×K	926.93	Joback Method
dvisc	0.0008664	Pa×s	443.92	Joback Method
dvisc	0.0006705	Pa×s	484.92	Joback Method

dvisc	0.0005401	Pa×s	525.91	Joback Method
dvisc	0.0004489	Pa×s	566.91	Joback Method
dvisc	0.0003825	Pa×s	607.91	Joback Method
dvisc	0.0003325	Pa×s	648.90	Joback Method
dvisc	0.0002940	Pa×s	689.90	Joback Method

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2395973&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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