ANTHRACENE, 1,4-DIMETHYL-

Inchi: InChI=1S/C16H14/c1-11-7-8-12(2)16-10-14-6-4-3-5-13(14)9-15(11)16/h3-10H,1-2H3
InchiKey: VQBRTNVYEIZVMP-UHFFFAOYSA-N
Formula: C16H14
SMILES: Cc1ccc(C)c2cc3ccccc3cc12
Mol. weight [g/mol]: 206.29

Physical Properties

Property code	Value	Unit	Source
af	0.5160		Cheméo Relay (1.0)
gf	380.66	kJ/mol	Joback Method
hf	162.34	kJ/mol	Cheméo Relay (1.0)
hfus	24.11	kJ/mol	Joback Method
hvap	90.35	kJ/mol	Cheméo Relay (1.0)
ie	7.22	eV	Cheméo Relay (1.0)
log10ws	-6.42		Cheméo Relay (1.0)
logp	4.610		Crippen Method
mcvol	173.620	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
tb	646.76	K	Cheméo Relay (1.0)
tc	893.20	K	Cheméo Relay (1.0)
tf	444.47	K	Cheméo Relay (1.0)
vc	0.652	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.69	J/mol×K	645.06	Joback Method
cpg	445.30	J/mol×K	685.83	Joback Method
cpg	459.74	J/mol×K	726.60	Joback Method
cpg	473.15	J/mol×K	767.36	Joback Method
cpg	485.63	J/mol×K	808.13	Joback Method
cpg	497.31	J/mol×K	848.90	Joback Method
cpg	508.31	J/mol×K	889.67	Joback Method
dvisc	0.0012344	Pa×s	399.46	Joback Method

dvisc	0.0009553	Pa×s	440.39	Joback Method
dvisc	0.0007722	Pa×s	481.33	Joback Method
dvisc	0.0006454	Pa×s	522.26	Joback Method
dvisc	0.0005537	Pa×s	563.19	Joback Method
dvisc	0.0004850	Pa×s	604.13	Joback Method
dvisc	0.0004320	Pa×s	645.06	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C781920&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
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