ANTHRACENE, 9-(1-METHYLETHYL)-

Inchi: InChI=1S/C17H16/c1-12(2)17-15-9-5-3-7-13(15)11-14-8-4-6-10-16(14)17/h3-12H,1-2H3
InchiKey: LQRJPEHNMOASNZ-UHFFFAOYSA-N
Formula: C17H16
SMILES: CC(C)c1c2ccccc2cc2ccccc12
Mol. weight [g/mol]: 220.32

Physical Properties

Property code	Value	Unit	Source
af	0.5000		Cheméo Relay (1.0)
gf	396.27	kJ/mol	Joback Method
hf	140.21	kJ/mol	Cheméo Relay (1.0)
hfus	23.56	kJ/mol	Joback Method
hvap	88.50	kJ/mol	Cheméo Relay (1.0)
ie	7.41	eV	Cheméo Relay (1.0)
log10ws	-6.18		Cheméo Relay (1.0)
logp	5.116		Crippen Method
mcvol	187.710	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
tb	639.51	K	Cheméo Relay (1.0)
tc	893.80	K	Cheméo Relay (1.0)
tf	369.67	K	Cheméo Relay (1.0)
vc	0.694	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.75	J/mol×K	662.52	Joback Method
cpg	498.45	J/mol×K	703.11	Joback Method
cpg	513.88	J/mol×K	743.71	Joback Method
cpg	528.20	J/mol×K	784.30	Joback Method
cpg	541.51	J/mol×K	824.90	Joback Method
cpg	553.97	J/mol×K	865.49	Joback Method
cpg	565.69	J/mol×K	906.08	Joback Method
dvisc	0.0015596	Pa×s	383.21	Joback Method

dvisc	0.0010847	Pa×s	429.76	Joback Method
dvisc	0.0008099	Pa×s	476.31	Joback Method
dvisc	0.0006370	Pa×s	522.87	Joback Method
dvisc	0.0005210	Pa×s	569.42	Joback Method
dvisc	0.0004394	Pa×s	615.97	Joback Method
dvisc	0.0003795	Pa×s	662.52	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1498802&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