ACEPHENANTHRYLENE, 4,5-DIHYDRO-

Other names: 4,5-Dihydroacephenanthrylene
Inchi: InChI=1S/C16H12/c1-2-6-14-12(4-1)10-13-9-8-11-5-3-7-15(14)16(11)13/h1-7,10H,8-9H2
InchiKey: ZBWXZZIIMVVCNZ-UHFFFAOYSA-N
Formula: C16H12
SMILES: c1ccc2c(c1)cc1c3c(cccc32)CC1
Mol. weight [g/mol]: 204.27

Physical Properties

Property code	Value	Unit	Source
hf	240.31	kJ/mol	Cheméo Relay (1.0)
hfus	23.27	kJ/mol	Joback Method
hvap	93.31	kJ/mol	Cheméo Relay (1.0)
ie	7.58	eV	Cheméo Relay (1.0)
log10ws	-6.40		Cheméo Relay (1.0)
logp	4.092		Crippen Method
mcvol	162.760	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
tb	656.28	K	Cheméo Relay (1.0)
tc	932.24	K	Cheméo Relay (1.0)
tf	390.06	K	Cheméo Relay (1.0)
vc	0.646	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.09	J/mol×K	652.20	Joback Method
cpg	483.57	J/mol×K	905.80	Joback Method
cpg	472.96	J/mol×K	863.54	Joback Method
cpg	461.97	J/mol×K	821.27	Joback Method
cpg	450.39	J/mol×K	779.00	Joback Method
cpg	438.02	J/mol×K	736.73	Joback Method
cpg	424.65	J/mol×K	694.47	Joback Method
dvisc	0.0015468	Pa×s	538.68	Joback Method
dvisc	0.0012660	Pa×s	652.20	Joback Method

dvisc	0.0013423	Pa×s	614.36	Joback Method
dvisc	0.0014342	Pa×s	576.52	Joback Method
dvisc	0.0021032	Pa×s	425.16	Joback Method
dvisc	0.0016873	Pa×s	500.84	Joback Method
dvisc	0.0018669	Pa×s	463.00	Joback Method

Sources

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=C6232480&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

Legend

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