5,6-Dihydro-4H-benz[de]anthracene

Other names: 5,6-Dihydro-4H-benz[de]anthracene
Inchi: InChI=1S/C17H14/c1-2-9-15-13(5-1)11-14-8-3-6-12-7-4-10-16(15)17(12)14/h1-2,4-5,7,9-
InchiKey: VFZDNSWGNPSQLY-UHFFFAOYSA-N
Formula: C17H14
SMILES: c1ccc2c(c1)cc1c3c(cccc32)CCC1
Mol. weight [g/mol]: 218.30

Physical Properties

Property code	Value	Unit	Source
af	0.5261		Cheméo Relay (1.0)
hf	189.41	kJ/mol	Cheméo Relay (1.0)
hfus	23.76	kJ/mol	Joback Method
hvap	95.81	kJ/mol	Cheméo Relay (1.0)
ie	7.63	eV	Cheméo Relay (1.0)
log10ws	-6.37		Cheméo Relay (1.0)
logp	4.482		Crippen Method
mcvol	176.850	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
tb	668.14	K	Cheméo Relay (1.0)
tc	944.33	K	Cheméo Relay (1.0)
tf	353.60 ± 1.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.24	J/mol×K	679.35	Joback Method
cpg	478.18	J/mol×K	722.05	Joback Method
cpg	492.87	J/mol×K	764.75	Joback Method
cpg	506.49	J/mol×K	807.45	Joback Method
cpg	519.26	J/mol×K	850.15	Joback Method
cpg	531.38	J/mol×K	892.86	Joback Method
cpg	543.05	J/mol×K	935.56	Joback Method
dvisc	0.0020061	Pa×s	432.91	Joback Method
dvisc	0.0016661	Pa×s	473.98	Joback Method

dvisc	0.0014254	Pa×s	515.06	Joback Method
dvisc	0.0012479	Pa×s	556.13	Joback Method
dvisc	0.0011126	Pa×s	597.20	Joback Method
dvisc	0.0010068	Pa×s	638.28	Joback Method
dvisc	0.0009221	Pa×s	679.35	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4389097&Units=SI

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