CYCLOBUT[A]ACENAPHTHYLENE, 6B,8A-DIHYDRO-

Inchi: InChI=1S/C14H10/c1-3-9-4-2-6-13-11-8-7-10(11)12(5-1)14(9)13/h1-8,10-11H
InchiKey: MKRSLSRLZZVPKE-UHFFFAOYSA-N
Formula: C14H10
SMILES: C1=CC2c3cccc4cccc(c34)C12
Mol. weight [g/mol]: 178.23

Physical Properties

Property code	Value	Unit	Source
hf	382.42	kJ/mol	Cheméo Relay (1.0)
hfus	23.99	kJ/mol	Joback Method
hvap	74.20	kJ/mol	Cheméo Relay (1.0)
ie	7.72	eV	NIST Webbook
log10ws	-4.69		Cheméo Relay (1.0)
logp	3.590		Crippen Method
mcvol	138.880	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
tb	572.06	K	Cheméo Relay (1.0)
tc	851.10	K	Cheméo Relay (1.0)
tf	345.85	K	Cheméo Relay (1.0)
vc	0.553	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.08	J/mol×K	579.44	Joback Method
cpg	353.67	J/mol×K	619.97	Joback Method
cpg	366.91	J/mol×K	660.50	Joback Method
cpg	379.00	J/mol×K	701.03	Joback Method
cpg	390.13	J/mol×K	741.56	Joback Method
cpg	400.48	J/mol×K	782.09	Joback Method
cpg	410.24	J/mol×K	822.62	Joback Method
dvisc	0.0019051	Pa×s	375.38	Joback Method
dvisc	0.0020324	Pa×s	409.39	Joback Method
dvisc	0.0021467	Pa×s	443.40	Joback Method

dvisc	0.0022499	Pa×s	477.41	Joback Method
dvisc	0.0023433	Pa×s	511.42	Joback Method
dvisc	0.0024283	Pa×s	545.43	Joback Method
dvisc	0.0025059	Pa×s	579.44	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=C30736799&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