6H-Dibenzo[b,d]pyrane

Other names: 6H-Dibenzo[b,d]pyrane
Inchi: InChI=1S/C13H10O/c1-2-6-11-10(5-1)9-14-13-8-4-3-7-12(11)13/h1-8H,9H2
InchiKey: BEUDCHGZCTUAOG-UHFFFAOYSA-N
Formula: C13H10O
SMILES: c1ccc2c(c1)COc1ccccc1-2
Mol. weight [g/mol]: 182.22

Physical Properties

Property code	Value	Unit	Source
hf	72.20	kJ/mol	Cheméo Relay (1.0)
hfus	23.87	kJ/mol	Joback Method
hvap	80.28	kJ/mol	Cheméo Relay (1.0)
ie	7.67	eV	Cheméo Relay (1.0)
log10ws	-4.62		Cheméo Relay (1.0)
logp	3.246		Crippen Method
mcvol	141.520	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
tb	580.67	K	Cheméo Relay (1.0)
tc	859.19	K	Cheméo Relay (1.0)
tf	357.64	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.88	J/mol×K	594.25	Joback Method
cpg	407.26	J/mol×K	847.39	Joback Method
cpg	397.69	J/mol×K	805.20	Joback Method
cpg	387.36	J/mol×K	763.01	Joback Method
cpg	376.14	J/mol×K	720.82	Joback Method
cpg	363.91	J/mol×K	678.63	Joback Method
cpg	350.54	J/mol×K	636.44	Joback Method
dvisc	0.0008043	Pa×s	480.34	Joback Method
dvisc	0.0004895	Pa×s	594.25	Joback Method
dvisc	0.0005647	Pa×s	556.28	Joback Method

dvisc	0.0006653	Pa×s	518.31	Joback Method
dvisc	0.0017995	Pa×s	366.42	Joback Method
dvisc	0.0010046	Pa×s	442.36	Joback Method
dvisc	0.0013082	Pa×s	404.39	Joback Method

Sources

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=C229958&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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