

4H-Cyclopenta[def]triphenylene

Inchi: InChI=1S/C19H12/c1-2-8-15-14(7-1)16-9-3-5-12-11-13-6-4-10-17(15)19(13)18(12)16/h1-12
InchiKey: OQXWDZOQDYGDAB-UHFFFAOYSA-N
Formula: C19H12
SMILES: c1ccc2c(c1)c1cccc3c1c1c(cccc21)C3
Mol. weight [g/mol]: 240.31

Physical Properties

Property code	Value	Unit	Source
hf	315.02	kJ/mol	Cheméo Relay (1.0)
hfus	29.77	kJ/mol	Joback Method
hvap	112.76	kJ/mol	Cheméo Relay (1.0)
ie	7.58	eV	Cheméo Relay (1.0)
log10ws	-7.58		Cheméo Relay (1.0)
logp	5.050		Crippen Method
mcvol	185.570	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
tb	735.45	K	Cheméo Relay (1.0)
tc	1024.50	K	Cheméo Relay (1.0)
tf	458.18	K	Cheméo Relay (1.0)
vc	0.744	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.08	J/mol×K	740.53	Joback Method
cpg	566.02	J/mol×K	999.94	Joback Method
cpg	553.80	J/mol×K	956.70	Joback Method
cpg	541.90	J/mol×K	913.47	Joback Method
cpg	530.06	J/mol×K	870.23	Joback Method
cpg	517.99	J/mol×K	827.00	Joback Method
cpg	505.43	J/mol×K	783.76	Joback Method
dvisc	0.0033565	Pa×s	624.12	Joback Method
dvisc	0.0030808	Pa×s	740.53	Joback Method
dvisc	0.0031601	Pa×s	701.73	Joback Method

dvisc	0.0032511	Pa×s	662.92	Joback Method
dvisc	0.0038035	Pa×s	507.71	Joback Method
dvisc	0.0034800	Pa×s	585.32	Joback Method
dvisc	0.0036267	Pa×s	546.51	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=C23992327&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
vc:	Critical Volume

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