2,5-DIPHENYL-CYCLOPROPABENZENE

Other names: 2,5-Diphenyl-cyclopropabenzene
Inchi: InChI=1S/C19H14/c1-3-7-14(8-4-1)16-11-12-17(19-13-18(16)19)15-9-5-2-6-10-15/h1-12H
InchiKey: GWDDTHGMCIPFBE-UHFFFAOYSA-N
Formula: C19H14
SMILES: c1ccc(-c2ccc(-c3ccccc3)c3c2C3)cc1
Mol. weight [g/mol]: 242.32

Physical Properties

Property code	Value	Unit	Source
af	0.5266		Cheméo Relay (1.0)
gf	510.10	kJ/mol	Joback Method
hf	361.28	kJ/mol	Cheméo Relay (1.0)
hfus	27.19	kJ/mol	Joback Method
hvap	108.16	kJ/mol	Cheméo Relay (1.0)
ie	7.98	eV	Cheméo Relay (1.0)
log10ws	-7.04		Cheméo Relay (1.0)
logp	4.925		Crippen Method
mcvol	196.430	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
tb	678.36	K	Cheméo Relay (1.0)
tc	941.50	K	Cheméo Relay (1.0)
tf	434.31	K	Cheméo Relay (1.0)
vc	0.760	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.47	J/mol×K	731.97	Joback Method
cpg	538.55	J/mol×K	776.25	Joback Method
cpg	553.34	J/mol×K	820.53	Joback Method
cpg	567.05	J/mol×K	864.81	Joback Method
cpg	579.88	J/mol×K	909.09	Joback Method
cpg	592.05	J/mol×K	953.38	Joback Method
cpg	603.77	J/mol×K	997.66	Joback Method

dvisc	0.0015665	Pa×s	449.93	Joback Method
dvisc	0.0011792	Pa×s	496.94	Joback Method
dvisc	0.0009323	Pa×s	543.94	Joback Method
dvisc	0.0007651	Pa×s	590.95	Joback Method
dvisc	0.0006465	Pa×s	637.96	Joback Method
dvisc	0.0005591	Pa×s	684.96	Joback Method
dvisc	0.0004925	Pa×s	731.97	Joback Method

Sources

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=C52750126&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
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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