

PHENANTHRENE, 2-PHENYL-

Other names:	2-Phenylphenanthrene
Inchi:	InChI=1S/C20H14/c1-2-6-15(7-3-1)17-12-13-20-18(14-17)11-10-16-8-4-5-9-19(16)20/h1-
InchiKey:	OSOLELDZBFOFHO-UHFFFAOYSA-N
Formula:	C20H14
SMILES:	c1ccc(-c2ccc3c(ccc4ccccc43)c2)cc1
Mol. weight [g/mol]:	254.33

Physical Properties

Property code	Value	Unit	Source
af	0.5324		Cheméo Relay (1.0)
gf	536.38	kJ/mol	Joback Method
hf	339.63	kJ/mol	Cheméo Relay (1.0)
hfus	28.90	kJ/mol	Joback Method
hvap	114.76	kJ/mol	Cheméo Relay (1.0)
ie	7.54	eV	Cheméo Relay (1.0)
log10ws	-7.62		Cheméo Relay (1.0)
logp	5.660		Crippen Method
mcvol	206.220	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
rinpol	424.19		NIST Webbook
rinpol	424.19		NIST Webbook
tb	727.20	K	Cheméo Relay (1.0)
tc	1006.99	K	Cheméo Relay (1.0)
tf	421.75	K	Cheméo Relay (1.0)
vc	0.781	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.94	J/mol×K	758.28	Joback Method
cpg	633.72	J/mol×K	1028.40	Joback Method
cpg	622.13	J/mol×K	983.38	Joback Method
cpg	610.08	J/mol×K	938.36	Joback Method
cpg	597.34	J/mol×K	893.34	Joback Method

cpg	583.72	J/mol×K	848.32	Joback Method
cpg	568.99	J/mol×K	803.30	Joback Method
dvisc	0.0005812	Pa×s	608.36	Joback Method
dvisc	0.0003497	Pa×s	758.28	Joback Method
dvisc	0.0004045	Pa×s	708.31	Joback Method
dvisc	0.0004782	Pa×s	658.33	Joback Method
dvisc	0.0013464	Pa×s	458.44	Joback Method
dvisc	0.0007314	Pa×s	558.39	Joback Method
dvisc	0.0009631	Pa×s	508.41	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=C4325773&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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