

1-phenylphenanthrene

Inchi:	InChI=1S/C20H14/c1-2-7-15(8-3-1)18-11-6-12-19-17-10-5-4-9-16(17)13-14-20(18)19/h1-
InchiKey:	RKLROMDZXDQSDF-UHFFFAOYSA-N
Formula:	C20H14
SMILES:	<chem>c1ccc(-c2cccc3c2ccc2ccccc23)cc1</chem>
Mol. weight [g/mol]:	254.33

Physical Properties

Property code	Value	Unit	Source
gf	536.38	kJ/mol	Joback Method
hf	376.13	kJ/mol	Joback Method
hfus	28.90	kJ/mol	Joback Method
hvap	69.27	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	5.660		Crippen Method
mcvol	206.220	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
rinpol	421.66		NIST Webbook
rinpol	421.66		NIST Webbook
rinpol	421.66		NIST Webbook
rinpol	421.96		NIST Webbook
rinpol	421.17		NIST Webbook
tb	758.28	K	Joback Method
tc	1028.40	K	Joback Method
tf	458.44	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.94	J/molxK	758.28	Joback Method
cpg	568.99	J/molxK	803.30	Joback Method
cpg	583.72	J/molxK	848.32	Joback Method
cpg	597.34	J/molxK	893.34	Joback Method
cpg	610.08	J/molxK	938.36	Joback Method

cpg	622.13	J/mol×K	983.38	Joback Method
cpg	633.72	J/mol×K	1028.40	Joback Method
dvisc	0.0013464	Paxs	458.44	Joback Method
dvisc	0.0009631	Paxs	508.41	Joback Method
dvisc	0.0007314	Paxs	558.39	Joback Method
dvisc	0.0005812	Paxs	608.36	Joback Method
dvisc	0.0004782	Paxs	658.33	Joback Method
dvisc	0.0004045	Paxs	708.31	Joback Method
dvisc	0.0003497	Paxs	758.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R15486&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
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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