

Phenanthrene, 9-methyl-10-phenyl

Inchi:	InChI=1S/C21H16/c1-15-17-11-5-6-12-18(17)19-13-7-8-14-20(19)21(15)16-9-3-2-4-10-1
InchiKey:	VASMZEZNNVGPBU-UHFFFAOYSA-N
Formula:	C21H16
SMILES:	Cc1c(-c2ccccc2)c2ccccc2c2ccccc12
Mol. weight [g/mol]:	268.35

Physical Properties

Property code	Value	Unit	Source
gf	535.17	kJ/mol	Joback Method
hf	344.02	kJ/mol	Joback Method
hfus	31.10	kJ/mol	Joback Method
hvap	72.16	kJ/mol	Joback Method
log10ws	-8.16		Crippen Method
logp	5.968		Crippen Method
mcvol	220.310	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
tb	786.14	K	Joback Method
tc	1050.54	K	Joback Method
tf	482.23	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.85	J/molxK	786.14	Joback Method
cpg	622.09	J/molxK	830.21	Joback Method
cpg	637.11	J/molxK	874.27	Joback Method
cpg	651.11	J/molxK	918.34	Joback Method
cpg	664.28	J/molxK	962.41	Joback Method
cpg	676.81	J/molxK	1006.47	Joback Method
cpg	688.89	J/molxK	1050.54	Joback Method
dvisc	0.0011816	Paxs	482.23	Joback Method
dvisc	0.0008610	Paxs	532.88	Joback Method
dvisc	0.0006629	Paxs	583.53	Joback Method

dvisc	0.0005321	Paxs	634.19	Joback Method
dvisc	0.0004412	Paxs	684.84	Joback Method
dvisc	0.0003754	Paxs	735.49	Joback Method
dvisc	0.0003262	Paxs	786.14	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R215540&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i

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
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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