

9-methyl-10-ethylphenanthrene

Other names:	Phenanthrene, 9-ethyl-10-methyl
Inchi:	InChI=1S/C17H16/c1-3-13-12(2)14-8-4-5-10-16(14)17-11-7-6-9-15(13)17/h4-11H,3H2,1-
InchiKey:	KEJXNUMQLIPTIV-UHFFFAOYSA-N
Formula:	C17H16
SMILES:	CCc1c(C)c2ccccc2c2ccccc12
Mol. weight [g/mol]:	220.31

Physical Properties

Property code	Value	Unit	Source
gf	389.08	kJ/mol	Joback Method
hf	190.05	kJ/mol	Joback Method
hfus	26.70	kJ/mol	Joback Method
hvap	60.98	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	4.864		Crippen Method
mcvol	187.710	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
rinpol	359.91		NIST Webbook
rinpol	360.73		NIST Webbook
rinpol	360.73		NIST Webbook
rinpol	359.91		NIST Webbook
tb	667.94	K	Joback Method
tc	907.34	K	Joback Method
tf	410.73	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.42	J/mol×K	667.94	Joback Method
cpg	496.53	J/mol×K	707.84	Joback Method
cpg	511.50	J/mol×K	747.74	Joback Method
cpg	525.45	J/mol×K	787.64	Joback Method
cpg	538.48	J/mol×K	827.54	Joback Method

cpg	550.72	J/mol×K	867.44	Joback Method
cpg	562.29	J/mol×K	907.34	Joback Method
dvisc	0.0012598	Pa×s	410.73	Joback Method
dvisc	0.0009568	Pa×s	453.60	Joback Method
dvisc	0.0007620	Pa×s	496.47	Joback Method
dvisc	0.0006292	Pa×s	539.34	Joback Method
dvisc	0.0005345	Pa×s	582.20	Joback Method
dvisc	0.0004643	Pa×s	625.07	Joback Method
dvisc	0.0004106	Pa×s	667.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R15561&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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