9,10-Dimethyl-3-ethylphenanthrene

Other names: Phenanthrene, 3-ethyl-9,10-dimethyl
Inchi: InChI=1S/C18H18/c1-4-14-9-10-16-13(3)12(2)15-7-5-6-8-17(15)18(16)11-14/h5-11H,4H2
InchiKey: DRJPELPJTRKFDF-UHFFFAOYSA-N
Formula: C18H18
SMILES: CCc1ccc2c(C)c(C)c3ccccc3c2c1
Mol. weight [g/mol]: 234.34

Physical Properties

Property code	Value	Unit	Source
gf	387.87	kJ/mol	Joback Method
hf	157.94	kJ/mol	Joback Method
hfus	28.90	kJ/mol	Joback Method
hvap	63.87	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	5.172		Crippen Method
mcvol	201.800	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	381.85		NIST Webbook
rinpol	381.85		NIST Webbook
rinpol	381.70		NIST Webbook
rinpol	381.70		NIST Webbook
tb	695.80	K	Joback Method
tc	931.19	K	Joback Method
tf	434.52	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.64	J/mol×K	695.80	Joback Method
cpg	603.81	J/mol×K	891.96	Joback Method
cpg	591.11	J/mol×K	852.73	Joback Method
cpg	577.64	J/mol×K	813.50	Joback Method
cpg	563.32	J/mol×K	774.26	Joback Method

cpg	548.02	J/mol×K	735.03	Joback Method
cpg	615.85	J/mol×K	931.19	Joback Method
dvisc	0.0003893	Pa×s	695.80	Joback Method
dvisc	0.0004384	Pa×s	652.25	Joback Method
dvisc	0.0005022	Pa×s	608.71	Joback Method
dvisc	0.0005875	Pa×s	565.16	Joback Method
dvisc	0.0007054	Pa×s	521.61	Joback Method
dvisc	0.0008758	Pa×s	478.07	Joback Method
dvisc	0.0011354	Pa×s	434.52	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R15557&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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