9,10-diethylphenanthrene

Other names: Phenanthrene, 9,10-diethyl
Inchi: InChI=1S/C18H18/c1-3-13-14(4-2)16-10-6-8-12-18(16)17-11-7-5-9-15(13)17/h5-12H,3-4
InchiKey: JURXVMQHSBALPL-UHFFFAOYSA-N
Formula: C18H18
SMILES: CCc1c(CC)c2ccccc2c2ccccc12
Mol. weight [g/mol]: 234.34

Physical Properties

Property code	Value	Unit	Source
gf	397.50	kJ/mol	Joback Method
hf	169.41	kJ/mol	Joback Method
hfus	29.29	kJ/mol	Joback Method
hvap	63.20	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	5.118		Crippen Method
mcvol	201.800	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinpol	367.70		NIST Webbook
rinpol	367.97		NIST Webbook
rinpol	367.97		NIST Webbook
rinpol	367.97		NIST Webbook
rinpol	367.70		NIST Webbook
tb	690.82	K	Joback Method
tc	925.38	K	Joback Method
tf	422.00	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.49	J/mol×K	690.82	Joback Method
cpg	549.03	J/mol×K	729.91	Joback Method
cpg	564.45	J/mol×K	769.01	Joback Method
cpg	578.86	J/mol×K	808.10	Joback Method

cpg	592.37	J/mol×K	847.19	Joback Method
cpg	605.10	J/mol×K	886.28	Joback Method
cpg	617.17	J/mol×K	925.38	Joback Method
dvisc	0.0012700	Pa×s	422.00	Joback Method
dvisc	0.0009471	Pa×s	466.80	Joback Method
dvisc	0.0007436	Pa×s	511.61	Joback Method
dvisc	0.0006069	Pa×s	556.41	Joback Method
dvisc	0.0005107	Pa×s	601.21	Joback Method
dvisc	0.0004401	Pa×s	646.02	Joback Method
dvisc	0.0003866	Pa×s	690.82	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R15543&Units=SI

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

Latest version available from: