Phenanthrene, 4-ethyl

Other names: 4-ethyl-Phenanthrene
Inchi: InChI=1S/C16H14/c1-2-12-7-5-8-14-11-10-13-6-3-4-9-15(13)16(12)14/h3-11H,2H2,1H3
InchiKey: PPCUEIMOKCJWOK-UHFFFAOYSA-N
Formula: C16H14
SMILES: CCc1cccc2ccc3ccccc3c12
Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
gf	390.29	kJ/mol	Joback Method
hf	222.16	kJ/mol	Joback Method
hfus	24.50	kJ/mol	Joback Method
hvap	58.09	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.555		Crippen Method
mcvol	173.620	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	331.74		NIST Webbook
rinpol	331.60		NIST Webbook
rinpol	331.59		NIST Webbook
tb	640.08	K	Joback Method
tc	883.76	K	Joback Method
tf	386.94	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.53	J/mol×K	640.08	Joback Method
cpg	498.83	J/mol×K	843.15	Joback Method
cpg	487.10	J/mol×K	802.53	Joback Method
cpg	474.53	J/mol×K	761.92	Joback Method
cpg	461.00	J/mol×K	721.31	Joback Method
cpg	446.38	J/mol×K	680.69	Joback Method

cpg	509.85	J/mol×K	883.76	Joback Method
dvisc	0.0004317	Pa×s	640.08	Joback Method
dvisc	0.0004902	Pa×s	597.89	Joback Method
dvisc	0.0005675	Pa×s	555.70	Joback Method
dvisc	0.0006730	Pa×s	513.51	Joback Method
dvisc	0.0008227	Pa×s	471.32	Joback Method
dvisc	0.0010464	Pa×s	429.13	Joback Method
dvisc	0.0014025	Pa×s	386.94	Joback Method

Sources

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=R67663&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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