1,4-dimethylphenanthrene

Other names: Phenanthrene, 1,4-dimethyl-
Inchi: InChI=1S/C16H14/c1-11-7-8-12(2)16-14(11)10-9-13-5-3-4-6-15(13)16/h3-10H,1-2H3
InchiKey: DWMAJXVIIUYYOH-UHFFFAOYSA-N
Formula: C16H14
SMILES: Cc1ccc(C)c2c1ccc1ccccc12
Mol. weight [g/mol]: 206.28
CAS: 22349-59-3

Physical Properties

Property code	Value	Unit	Source
gf	380.66	kJ/mol	Joback Method
hf	210.69	kJ/mol	Joback Method
hfus	24.11	kJ/mol	Joback Method
hvap	58.75	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	4.610		Crippen Method
mcvol	173.620	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	344.00		NIST Webbook
rinpol	344.09		NIST Webbook
rinpol	344.00		NIST Webbook
tb	645.06	K	Joback Method
tc	889.67	K	Joback Method
tf	324.00 ± 2.00	K	NIST Webbook
tf	322.90 ± 0.70	K	NIST Webbook
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.69	J/mol×K	645.06	Joback Method
cpg	445.30	J/mol×K	685.83	Joback Method
cpg	459.74	J/mol×K	726.60	Joback Method
cpg	473.15	J/mol×K	767.36	Joback Method

cpg	485.63	J/mol×K	808.13	Joback Method
cpg	497.31	J/mol×K	848.90	Joback Method
cpg	508.31	J/mol×K	889.67	Joback Method
dvisc	0.0012344	Pa×s	399.46	Joback Method
dvisc	0.0009553	Pa×s	440.39	Joback Method
dvisc	0.0007722	Pa×s	481.33	Joback Method
dvisc	0.0006454	Pa×s	522.26	Joback Method
dvisc	0.0005537	Pa×s	563.19	Joback Method
dvisc	0.0004850	Pa×s	604.13	Joback Method
dvisc	0.0004320	Pa×s	645.06	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=C22349593&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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