

Naphth[2,3-e]acephenanthrylene

Inchi:	InChI=1S/C24H14/c1-2-7-16-13-22-21(12-15(16)6-1)20-11-5-10-19-18-9-4-3-8-17(18)14
InchiKey:	JKKWIMTZWPKTTI-UHFFFAOYSA-N
Formula:	C24H14
SMILES:	c1ccc2cc3c(cc2c1)-c1cccc2c1c-3cc1ccccc12
Mol. weight [g/mol]:	302.37
CAS:	205-97-0

Physical Properties

Property code	Value	Unit	Source
gf	752.58	kJ/mol	Joback Method
hf	561.85	kJ/mol	Joback Method
hfus	38.47	kJ/mol	Joback Method
hvap	81.51	kJ/mol	Joback Method
log10ws	-10.34		Crippen Method
logp	6.794		Crippen Method
mcvol	232.260	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
tb	882.32	K	Joback Method
tc	1151.38	K	Joback Method
tf	606.52	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.66	J/mol×K	882.32	Joback Method
cpg	676.44	J/mol×K	927.16	Joback Method
cpg	691.24	J/mol×K	972.01	Joback Method
cpg	706.42	J/mol×K	1016.85	Joback Method
cpg	722.35	J/mol×K	1061.69	Joback Method
cpg	739.36	J/mol×K	1106.54	Joback Method
cpg	757.84	J/mol×K	1151.38	Joback Method
dvisc	0.0052883	Pa×s	606.52	Joback Method
dvisc	0.0049439	Pa×s	652.49	Joback Method

dvisc	0.0046630	Pa×s	698.45	Joback Method
dvisc	0.0044300	Pa×s	744.42	Joback Method
dvisc	0.0042338	Pa×s	790.39	Joback Method
dvisc	0.0040664	Pa×s	836.35	Joback Method
dvisc	0.0039222	Pa×s	882.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C205970&Units=SI&Mask=3FFF
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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