

1-(2-Naphthyl)-2-(3-phenathryl)ethylene, trans

Inchi:

IXFZYKXJNSHZOG-MDZDMXLPSA-N

InchiKey:

C26H18

Formula:

C(=Cc1ccc2ccc3ccccc3c2c1)c1ccc2ccccc2c1

SMILES:

330.42

Mol. weight [g/mol]:

Physical Properties

Property code	Value	Unit	Source
gf	764.14	kJ/mol	Joback Method
hf	549.11	kJ/mol	Joback Method
hfus	41.27	kJ/mol	Joback Method
hvap	84.89	kJ/mol	Joback Method
log10ws	-9.49		Crippen Method
logp	7.317		Crippen Method
mcvol	267.000	ml/mol	McGowan Method
pc	1874.03	kPa	Joback Method
rinpol	3640.00		NIST Webbook
rinpol	3640.00		NIST Webbook
tb	923.68	K	Joback Method
tc	1196.10	K	Joback Method
tf	566.20	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.31	J/mol×K	923.68	Joback Method
cpg	865.18	J/mol×K	1150.70	Joback Method
cpg	848.58	J/mol×K	1105.29	Joback Method
cpg	832.51	J/mol×K	1059.89	Joback Method
cpg	816.66	J/mol×K	1014.49	Joback Method
cpg	800.69	J/mol×K	969.08	Joback Method
cpg	882.62	J/mol×K	1196.10	Joback Method
dvisc	0.0003629	Pa×s	923.68	Joback Method

dvisc	0.0004137	Pa×s	864.10	Joback Method
dvisc	0.0004809	Pa×s	804.52	Joback Method
dvisc	0.0005725	Pa×s	744.94	Joback Method
dvisc	0.0007027	Pa×s	685.36	Joback Method
dvisc	0.0008967	Pa×s	625.78	Joback Method
dvisc	0.0012046	Pa×s	566.20	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=R525238&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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