1,2-bis-(3-phenathryl)ethylene, cis

Inchi: InChI=1S/C30H20/c1-3-7-27-23(5-1)15-17-25-13-11-21(19-29(25)27)9-10-22-12-14-26-1
InchiKey: YSPLDMAAYZIZAG-KTKRTIGZSA-N
Formula: C30H20
SMILES: C(=Cc1ccc2ccc3ccccc3c2c1)c1ccc2ccc3ccccc3c2c1
Mol. weight [g/mol]: 380.48

Physical Properties

Property code	Value	Unit	Source
gf	894.84	kJ/mol	Joback Method
hf	646.15	kJ/mol	Joback Method
hfus	48.26	kJ/mol	Joback Method
hvap	96.09	kJ/mol	Joback Method
log10ws	-11.29		Crippen Method
logp	8.470		Crippen Method
mcvol	303.900	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	3775.00		NIST Webbook
rinpol	3835.00		NIST Webbook
rinpol	3835.00		NIST Webbook
rinpol	3775.00		NIST Webbook
tb	1039.16	K	Joback Method
tc	1316.70	K	Joback Method
tf	656.50	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	939.95	J/mol×K	1039.16	Joback Method
cpg	958.86	J/mol×K	1085.42	Joback Method
cpg	978.39	J/mol×K	1131.67	Joback Method
cpg	998.95	J/mol×K	1177.93	Joback Method
cpg	1020.92	J/mol×K	1224.18	Joback Method
cpg	1044.70	J/mol×K	1270.44	Joback Method

cpg	1070.69	J/mol×K	1316.70	Joback Method
dvisc	0.0014379	Pa×s	656.50	Joback Method
dvisc	0.0011306	Pa×s	720.28	Joback Method
dvisc	0.0009244	Pa×s	784.05	Joback Method
dvisc	0.0007790	Pa×s	847.83	Joback Method
dvisc	0.0006724	Pa×s	911.61	Joback Method
dvisc	0.0005917	Pa×s	975.38	Joback Method
dvisc	0.0005289	Pa×s	1039.16	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=R525218&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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