1,2-bis-(2-Tetrahelicenyl)ethylene, cis

Inchi: InChI=1S/C38H24/c1-3-7-29-19-37-23-33-15-25(11-13-31(33)21-35(37)17-27(29)5-1)9-1
InchiKey: RSLYVBXLOJRYQE-KTKRTIGZSA-N
Formula: C38H24
SMILES: C(=Cc1ccc2cc3cc4ccccc4cc3cc2c1)c1ccc2cc3cc4ccccc4cc3cc2c1
Mol. weight [g/mol]: 480.60

Physical Properties

Property code	Value	Unit	Source
gf	1156.24	kJ/mol	Joback Method
hf	840.23	kJ/mol	Joback Method
hfus	62.24	kJ/mol	Joback Method
hvap	118.50	kJ/mol	Joback Method
log10ws	-14.90		Crippen Method
logp	10.776		Crippen Method
mcvol	377.700	ml/mol	McGowan Method
pc	1301.41	kPa	Joback Method
rinpol	5000.00		NIST Webbook
rinpol	5000.00		NIST Webbook
rinpol	5000.00		NIST Webbook
tb	1270.12	K	Joback Method
tc	1566.09	K	Joback Method
tf	837.10	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1306.20	J/mol×K	1270.12	Joback Method
cpg	1540.27	J/mol×K	1516.76	Joback Method
cpg	1482.54	J/mol×K	1467.43	Joback Method
cpg	1430.90	J/mol×K	1418.10	Joback Method
cpg	1384.71	J/mol×K	1368.78	Joback Method
cpg	1343.36	J/mol×K	1319.45	Joback Method
cpg	1604.72	J/mol×K	1566.09	Joback Method

dvisc	0.0011835	Pa×s	1270.12	Joback Method
dvisc	0.0012913	Pa×s	1197.95	Joback Method
dvisc	0.0014248	Pa×s	1125.78	Joback Method
dvisc	0.0015935	Pa×s	1053.61	Joback Method
dvisc	0.0018117	Pa×s	981.44	Joback Method
dvisc	0.0021022	Pa×s	909.27	Joback Method
dvisc	0.0025025	Pa×s	837.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R525203&Units=SI
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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