1,3,6,11-tetramethyl-triphenylene

Inchi: InChI=1S/C22H20/c1-13-5-7-17-18-8-6-14(2)11-20(18)22-16(4)9-15(3)12-21(22)19(17)10
InchiKey: VJSMOLXOGQALLK-UHFFFAOYSA-N
Formula: C22H20
SMILES: Cc1ccc2c3ccc(C)cc3c3c(C)cc(C)cc3c2c1
Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	508.94	kJ/mol	Joback Method
hf	243.51	kJ/mol	Joback Method
hfus	35.50	kJ/mol	Joback Method
hvap	75.73	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	6.380		Crippen Method
mcvol	238.700	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	461.72		NIST Webbook
rinpol	461.72		NIST Webbook
rinpol	461.72		NIST Webbook
tb	816.26	K	Joback Method
tc	1060.77	K	Joback Method
tf	537.34	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.35	J/mol×K	816.26	Joback Method
cpg	694.48	J/mol×K	857.01	Joback Method
cpg	709.74	J/mol×K	897.76	Joback Method
cpg	724.29	J/mol×K	938.51	Joback Method
cpg	738.27	J/mol×K	979.26	Joback Method
cpg	751.83	J/mol×K	1020.02	Joback Method
cpg	765.13	J/mol×K	1060.77	Joback Method

dvisc	0.0012783	Pa×s	537.34	Joback Method
dvisc	0.0010677	Pa×s	583.83	Joback Method
dvisc	0.0009157	Pa×s	630.31	Joback Method
dvisc	0.0008022	Pa×s	676.80	Joback Method
dvisc	0.0007147	Pa×s	723.29	Joback Method
dvisc	0.0006458	Pa×s	769.77	Joback Method
dvisc	0.0005903	Pa×s	816.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R15418&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

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