1,3-dimethyltriphenylene

Inchi: InChI=1S/C20H16/c1-13-11-14(2)20-18-10-6-5-8-16(18)15-7-3-4-9-17(15)19(20)12-13/h3
InchiKey: YQQFGIKMPKPSSR-UHFFFAOYSA-N
Formula: C20H16
SMILES: Cc1cc(C)c2c3ccccc3c3ccccc3c2c1
Mol. weight [g/mol]: 256.34

Physical Properties

Property code	Value	Unit	Source
gf	511.36	kJ/mol	Joback Method
hf	307.73	kJ/mol	Joback Method
hfus	31.10	kJ/mol	Joback Method
hvap	69.96	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	5.763		Crippen Method
mcvol	210.520	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	432.32		NIST Webbook
rinpol	432.32		NIST Webbook
rinpol	432.32		NIST Webbook
tb	760.54	K	Joback Method
tc	1013.66	K	Joback Method
tf	489.76	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.63	J/mol×K	760.54	Joback Method
cpg	639.81	J/mol×K	971.47	Joback Method
cpg	627.28	J/mol×K	929.28	Joback Method
cpg	614.28	J/mol×K	887.10	Joback Method
cpg	600.62	J/mol×K	844.91	Joback Method
cpg	586.13	J/mol×K	802.73	Joback Method
cpg	652.05	J/mol×K	1013.66	Joback Method

dvisc	0.0006539	Pa×s	760.54	Joback Method
dvisc	0.0007181	Pa×s	715.41	Joback Method
dvisc	0.0007987	Pa×s	670.28	Joback Method
dvisc	0.0009019	Pa×s	625.15	Joback Method
dvisc	0.0010381	Pa×s	580.02	Joback Method
dvisc	0.0012234	Pa×s	534.89	Joback Method
dvisc	0.0014862	Pa×s	489.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R15422&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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