1,3,6-Triphenylcycloheptatriene

Inchi: InChI=1S/C25H20/c1-4-10-20(11-5-1)23-16-17-24(21-12-6-2-7-13-21)19-25(18-23)22-14
InchiKey: GYYCHVGZUPXXKV-UHFFFAOYSA-N
Formula: C25H20
SMILES: C1=C(c2ccccc2)C=C(c2ccccc2)CC(c2ccccc2)=C1
Mol. weight [g/mol]: 320.43
CAS: 17760-68-8

Physical Properties

Property code	Value	Unit	Source
chs	-12970.00 ± 3.00	kJ/mol	NIST Webbook
gf	577.90	kJ/mol	Joback Method
hf	357.69	kJ/mol	Joback Method
hfs	274.00 ± 3.00	kJ/mol	NIST Webbook
hfus	33.79	kJ/mol	Joback Method
hvap	81.84	kJ/mol	Joback Method
log10ws	-7.55		Crippen Method
logp	6.641		Crippen Method
mcvol	268.070	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
tb	892.35	K	Joback Method
tc	1174.71	K	Joback Method
tf	498.71	K	Joback Method
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.98	J/mol×K	892.35	Joback Method
cpg	811.19	J/mol×K	939.41	Joback Method
cpg	826.58	J/mol×K	986.47	Joback Method
cpg	840.35	J/mol×K	1033.53	Joback Method
cpg	852.68	J/mol×K	1080.59	Joback Method
cpg	863.77	J/mol×K	1127.65	Joback Method
cpg	873.82	J/mol×K	1174.71	Joback Method

dvisc	0.0005202	Pa×s	498.71	Joback Method
dvisc	0.0002640	Pa×s	564.32	Joback Method
dvisc	0.0001543	Pa×s	629.92	Joback Method
dvisc	0.0000998	Pa×s	695.53	Joback Method
dvisc	0.0000696	Pa×s	761.14	Joback Method
dvisc	0.0000514	Pa×s	826.74	Joback Method
dvisc	0.0000397	Pa×s	892.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17760688&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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