Hexakis[(4-pentylphenyl)ethynyl]benzene

Inchi: InChI=1S/C84H90/c1-7-13-19-25-67-31-43-73(44-32-67)55-61-79-80(62-56-74-45-33-68
InchiKey: LTZVHPBZYRJACU-UHFFFAOYSA-N
Formula: C84H90
SMILES: CCCCCc1ccc(C#Cc2c(C#Cc3ccc(CCCCC)cc3)c(C#Cc3ccc(CCCCC)cc3)c(C#Cc3ccc(C
Mol. weight [g/mol]: 1099.61
CAS: 125594-05-0

Physical Properties

Property code	Value	Unit	Source
gf	2554.14	kJ/mol	Joback Method
hf	1386.25	kJ/mol	Joback Method
hfus	186.06	kJ/mol	Joback Method
hvap	238.70	kJ/mol	Joback Method
log10ws	-28.32		Crippen Method
logp	20.482		Crippen Method
mcvol	976.500	ml/mol	McGowan Method
pc	262.68	kPa	Joback Method
tb	2416.86	K	Joback Method
tc	4545.05	K	Joback Method
tf	1995.70	K	Joback Method
vc	3.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	4693.35	J/mol×K	2416.86	Joback Method
cpg	5885.64	J/mol×K	2771.56	Joback Method
cpg	7808.24	J/mol×K	3126.26	Joback Method
cpg	10666.48	J/mol×K	3480.95	Joback Method
cpg	14665.70	J/mol×K	3835.65	Joback Method
cpg	20011.22	J/mol×K	4190.35	Joback Method
cpg	26908.37	J/mol×K	4545.05	Joback Method
hfust	44.10	kJ/mol	443.55	NIST Webbook

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=C125594050&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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