Pentaphenyl benzene

Inchi: InChI=1S/C36H26/c1-6-16-27(17-7-1)32-26-33(28-18-8-2-9-19-28)35(30-22-12-4-13-23-3
InchiKey: JULFJTZPJNNMQK-UHFFFAOYSA-N
Formula: C36H26
SMILES: c1ccc(-c2cc(-c3ccccc3)c(-c3ccccc3)c(-c3ccccc3)c2-c2ccccc2)cc1
Mol. weight [g/mol]: 458.59
CAS: 18631-82-8

Physical Properties

Property code	Value	Unit	Source
gf	888.18	kJ/mol	Joback Method
hf	586.93	kJ/mol	Joback Method
hfus	51.69	kJ/mol	Joback Method
hvap	112.03	kJ/mol	Joback Method
log10ws	-14.49		Crippen Method
logp	10.022		Crippen Method
mcvol	375.540	ml/mol	McGowan Method
pc	1324.24	kPa	Joback Method
tb	1203.08	K	Joback Method
tc	1502.25	K	Joback Method
tf	704.08	K	Joback Method
vc	1.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1223.68	J/mol×K	1203.08	Joback Method
cpg	1238.09	J/mol×K	1252.94	Joback Method
cpg	1252.09	J/mol×K	1302.80	Joback Method
cpg	1266.01	J/mol×K	1352.66	Joback Method
cpg	1280.21	J/mol×K	1402.52	Joback Method
cpg	1295.04	J/mol×K	1452.38	Joback Method
cpg	1310.85	J/mol×K	1502.25	Joback Method
dvisc	0.0001288	Pa×s	704.08	Joback Method
dvisc	0.0000740	Pa×s	787.25	Joback Method

dvisc	0.0000473	Pa×s	870.41	Joback Method
dvisc	0.0000326	Pa×s	953.58	Joback Method
dvisc	0.0000239	Pa×s	1036.75	Joback Method
dvisc	0.0000184	Pa×s	1119.91	Joback Method
dvisc	0.0000146	Pa×s	1203.08	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=C18631828&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume