1,2,3,5,5 And 1,2,4,5,5-pentamethylcyclopentadiene mixture

Inchi: InChI=1S/C10H16/c1-7-6-10(4,5)9(3)8(7)2/h6H,1-5H3
InchiKey: ICWJGNMBERNILD-UHFFFAOYSA-N
Formula: C10H16
SMILES: CC1=CC(C)(C)C(C)=C1C
Mol. weight [g/mol]: 136.23
CAS: 41539-64-4

Physical Properties

Property code	Value	Unit	Source
gf	95.41	kJ/mol	Joback Method
hf	-92.86	kJ/mol	Joback Method
hfus	10.57	kJ/mol	Joback Method
hvap	39.53	kJ/mol	Joback Method
ie	7.77 ± 0.05	eV	NIST Webbook
log10ws	-3.37		Crippen Method
logp	3.309		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
tb	456.98	K	Joback Method
tc	662.70	K	Joback Method
tf	276.34	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.54	J/mol×K	456.98	Joback Method
cpg	290.57	J/mol×K	491.27	Joback Method
cpg	304.67	J/mol×K	525.55	Joback Method
cpg	317.94	J/mol×K	559.84	Joback Method
cpg	330.46	J/mol×K	594.13	Joback Method
cpg	342.32	J/mol×K	628.41	Joback Method
cpg	353.63	J/mol×K	662.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41539644&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
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
ie:	Ionization energy
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