2,4,5,7-Tetramethyl-4,5-bis(4-tert-butylphenyl)octa

Inchi: InChI=1S/C32H50/c1-23(2)21-31(11,27-17-13-25(14-18-27)29(5,6)7)32(12,22-24(3)4)28-
InchiKey: MFHJPQMOWKNBEO-UHFFFAOYSA-N
Formula: C32H50
SMILES: CC(C)CC(C)(c1ccc(C(C)(C)C)cc1)C(C)(CC(C)C)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 434.74
CAS: 85668-75-3

Physical Properties

Property code	Value	Unit	Source
chs	-19301.50 ± 4.80	kJ/mol	NIST Webbook
gf	430.60	kJ/mol	Joback Method
hf	-254.00 ± 5.40	kJ/mol	NIST Webbook
hfs	-436.60 ± 4.80	kJ/mol	NIST Webbook
hfus	29.24	kJ/mol	Joback Method
hsub	183.00	kJ/mol	NIST Webbook
hsub	182.60	kJ/mol	NIST Webbook
hvap	86.74	kJ/mol	Joback Method
log10ws	-9.57		Crippen Method
logp	9.589		Crippen Method
mcvol	414.220	ml/mol	McGowan Method
pc	786.39	kPa	Joback Method
tb	981.08	K	Joback Method
tc	1214.00	K	Joback Method
tf	507.96	K	Joback Method
vc	1.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1423.01	J/mol×K	981.08	Joback Method
cpg	1547.09	J/mol×K	1214.00	Joback Method
cpg	1527.34	J/mol×K	1175.18	Joback Method
cpg	1507.53	J/mol×K	1136.36	Joback Method
cpg	1487.41	J/mol×K	1097.54	Joback Method

cpg	1466.78	J/mol×K	1058.72	Joback Method
cpg	1445.39	J/mol×K	1019.90	Joback Method
cps	683.90	J/mol×K	298.00	NIST Webbook
dvisc	0.0000055	Pa×s	981.08	Joback Method
dvisc	0.0000081	Pa×s	902.23	Joback Method
dvisc	0.0000128	Pa×s	823.37	Joback Method
dvisc	0.0000223	Pa×s	744.52	Joback Method
dvisc	0.0000445	Pa×s	665.67	Joback Method
dvisc	0.0001065	Pa×s	586.81	Joback Method
dvisc	0.0003343	Pa×s	507.96	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C85668753&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase 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
hsub: Enthalpy of sublimation 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