4,5-Diethyl-4,5-bis-(4-tert-butylphenyl)-octane

Inchi: InChI=1S/C32H50/c1-11-23-31(13-3,27-19-15-25(16-20-27)29(5,6)7)32(14-4,24-12-2)28-
InchiKey: DTOQQIZHGNEYCR-UHFFFAOYSA-N
Formula: C32H50
SMILES: CCCC(CC)(c1ccc(C(C)(C)C)cc1)C(CC)(CCC)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 434.74
CAS: 85668-73-1

Physical Properties

Property code	Value	Unit	Source
chs	-19331.30 ± 3.50	kJ/mol	NIST Webbook
gf	435.48	kJ/mol	Joback Method
hf	-224.00 ± 4.60	kJ/mol	NIST Webbook
hfs	-406.80 ± 3.50	kJ/mol	NIST Webbook
hfus	36.28	kJ/mol	Joback Method
hsub	182.00	kJ/mol	NIST Webbook
hsub	182.80	kJ/mol	NIST Webbook
hvap	87.52	kJ/mol	Joback Method
log10ws	-10.05		Crippen Method
logp	9.878		Crippen Method
mcvol	414.220	ml/mol	McGowan Method
pc	779.38	kPa	Joback Method
tb	981.96	K	Joback Method
tc	1211.33	K	Joback Method
tf	537.96	K	Joback Method
vc	1.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1422.38	J/mol×K	981.96	Joback Method
cpg	1545.92	J/mol×K	1211.33	Joback Method
cpg	1526.18	J/mol×K	1173.10	Joback Method
cpg	1506.39	J/mol×K	1134.88	Joback Method
cpg	1486.34	J/mol×K	1096.65	Joback Method

cpg	1465.80	J/mol×K	1058.42	Joback Method
cpg	1444.56	J/mol×K	1020.19	Joback Method
cps	618.50	J/mol×K	298.00	NIST Webbook
dvisc	0.0000066	Pa×s	981.96	Joback Method
dvisc	0.0000094	Pa×s	907.96	Joback Method
dvisc	0.0000143	Pa×s	833.96	Joback Method
dvisc	0.0000235	Pa×s	759.96	Joback Method
dvisc	0.0000430	Pa×s	685.96	Joback Method
dvisc	0.0000909	Pa×s	611.96	Joback Method
dvisc	0.0002362	Pa×s	537.96	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=C85668731&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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