3,4-Diethyl-3,4-bis(4-tert-butylphenyl)-hexane

Inchi: InChI=1S/C30H46/c1-11-22(4)27(23-14-16-24(17-15-23)28(5,6)7)30(12-2,13-3)26-20-18
InchiKey: WNLBDFYTLIBLQU-UHFFFAOYSA-N
Formula: C30H46
SMILES: CCC(C)C(c1ccc(C(C)(C)C)cc1)C(CC)(CC)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 406.69
CAS: 85668-74-2

Physical Properties

Property code	Value	Unit	Source
chs	-18041.60 ± 1.30	kJ/mol	NIST Webbook
gf	410.92	kJ/mol	Joback Method
hf	-170.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-337.70 ± 1.30	kJ/mol	NIST Webbook
hfus	31.47	kJ/mol	Joback Method
hsub	168.00	kJ/mol	NIST Webbook
hsub	167.70	kJ/mol	NIST Webbook
hvap	83.59	kJ/mol	Joback Method
log10ws	-9.26		Crippen Method
logp	9.169		Crippen Method
mcvol	386.040	ml/mol	McGowan Method
pc	868.62	kPa	Joback Method
tb	938.55	K	Joback Method
tc	1166.04	K	Joback Method
tf	483.00	K	Joback Method
vc	1.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1410.49	J/mol×K	1166.04	Joback Method
cpg	1392.99	J/mol×K	1128.13	Joback Method
cpg	1375.03	J/mol×K	1090.21	Joback Method
cpg	1356.43	J/mol×K	1052.30	Joback Method
cpg	1337.02	J/mol×K	1014.38	Joback Method

cpg	1316.60	J/mol×K	976.47	Joback Method
cpg	1295.00	J/mol×K	938.55	Joback Method
cps	631.30	J/mol×K	298.00	NIST Webbook
dvisc	0.0000101	Pa×s	938.55	Joback Method
dvisc	0.0000146	Pa×s	862.62	Joback Method
dvisc	0.0000225	Pa×s	786.70	Joback Method
dvisc	0.0000382	Pa×s	710.77	Joback Method
dvisc	0.0000737	Pa×s	634.85	Joback Method
dvisc	0.0001696	Pa×s	558.92	Joback Method
dvisc	0.0005075	Pa×s	483.00	Joback Method
hfust	29.71	kJ/mol	400.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C85668742&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

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
hfust: Enthalpy of fusion at a given temperature
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