5,6-Dibutyl-5,6-bis(4-tert-butylphenyl)decane

Inchi: InChI=1S/C38H62/c1-11-15-27-37(28-16-12-2,33-23-19-31(20-24-33)35(5,6)7)38(29-17-
InchiKey: DMHYTJAITPRFFD-UHFFFAOYSA-N
Formula: C38H62
SMILES: CCCCC(CCCC)(c1ccc(C(C)(C)C)cc1)C(CCCC)(CCCC)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 518.90
CAS: 85668-76-4

Physical Properties

Property code	Value	Unit	Source
chs	-23242.70 ± 2.20	kJ/mol	NIST Webbook
gf	486.00	kJ/mol	Joback Method
hf	-351.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-571.30 ± 2.20	kJ/mol	NIST Webbook
hfus	51.82	kJ/mol	Joback Method
hsub	220.30	kJ/mol	NIST Webbook
hsub	221.00	kJ/mol	NIST Webbook
hvap	100.87	kJ/mol	Joback Method
log10ws	-12.56		Crippen Method
logp	12.218		Crippen Method
mcvol	498.760	ml/mol	McGowan Method
pc	578.40	kPa	Joback Method
tb	1119.24	K	Joback Method
tc	1372.31	K	Joback Method
tf	385.00 ± 1.00	K	NIST Webbook
vc	1.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1952.65	J/mol×K	1330.13	Joback Method
cpg	1821.98	J/mol×K	1119.24	Joback Method
cpg	1848.28	J/mol×K	1161.42	Joback Method
cpg	1874.17	J/mol×K	1203.60	Joback Method
cpg	1899.98	J/mol×K	1245.78	Joback Method

cpg	1926.03	J/mol×K	1287.95	Joback Method
cpg	1980.17	J/mol×K	1372.31	Joback Method
cps	805.50	J/mol×K	298.00	NIST Webbook
dvisc	0.0000023	Pa×s	1119.24	Joback Method
dvisc	0.0000899	Pa×s	605.58	Joback Method
dvisc	0.0000336	Pa×s	691.19	Joback Method
dvisc	0.0000156	Pa×s	776.80	Joback Method
dvisc	0.0000084	Pa×s	862.41	Joback Method
dvisc	0.0000051	Pa×s	948.02	Joback Method
dvisc	0.0000033	Pa×s	1033.63	Joback Method
hfust	43.10	kJ/mol	386.00	NIST Webbook

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=C85668764&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
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