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

Inchi: InChI=1S/C34H54/c1-11-23-33(24-12-2,29-19-15-27(16-20-29)31(5,6)7)34(25-13-3,26-1
InchiKey: JHALHDOCRWHJSQ-UHFFFAOYSA-N
Formula: C34H54
SMILES: CCCC(CCC)(c1ccc(C(C)(C)C)cc1)C(CCC)(CCC)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 462.79
CAS: 85668-72-0

Physical Properties

Property code	Value	Unit	Source
chs	-20686.00 ± 6.10	kJ/mol	NIST Webbook
gf	452.32	kJ/mol	Joback Method
hf	-213.00 ± 4.60	kJ/mol	NIST Webbook
hfs	-411.00 ± 6.10	kJ/mol	NIST Webbook
hfus	41.46	kJ/mol	Joback Method
hsub	198.00	kJ/mol	NIST Webbook
hsub	198.00	kJ/mol	NIST Webbook
hvap	91.97	kJ/mol	Joback Method
log10ws	-10.89		Crippen Method
logp	10.658		Crippen Method
mcvol	442.400	ml/mol	McGowan Method
pc	702.10	kPa	Joback Method
tb	1027.72	K	Joback Method
tc	1260.77	K	Joback Method
tf	419.00 ± 1.00	K	NIST Webbook
vc	1.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1662.74	J/mol×K	1221.93	Joback Method
cpg	1553.18	J/mol×K	1027.72	Joback Method
cpg	1576.17	J/mol×K	1066.56	Joback Method
cpg	1598.38	J/mol×K	1105.40	Joback Method
cpg	1620.05	J/mol×K	1144.25	Joback Method

cpg	1641.43	J/mol×K	1183.09	Joback Method
cpg	1684.23	J/mol×K	1260.77	Joback Method
cps	468.10	J/mol×K	393.00	NIST Webbook
cps	724.20	J/mol×K	298.00	NIST Webbook
dvisc	0.0000047	Pa×s	1027.72	Joback Method
dvisc	0.0001720	Pa×s	560.50	Joback Method
dvisc	0.0000655	Pa×s	638.37	Joback Method
dvisc	0.0000307	Pa×s	716.24	Joback Method
dvisc	0.0000167	Pa×s	794.11	Joback Method
dvisc	0.0000102	Pa×s	871.98	Joback Method
dvisc	0.0000067	Pa×s	949.85	Joback Method
hfust	36.11	kJ/mol	452.00	NIST Webbook
hfust	40.58	kJ/mol	419.00	NIST Webbook
sfust	79.90	J/mol×K	452.00	NIST Webbook

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=C85668720&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
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume