2,3-Dimethyl-2,3-bis(4-tert-butylphenyl)butane

Inchi: InChI=1S/C26H38/c1-23(2,3)19-11-15-21(16-12-19)25(7,8)26(9,10)22-17-13-20(14-18-2
InchiKey: VKUOFKIWVLOZFE-UHFFFAOYSA-N
Formula: C26H38
SMILES: CC(C)(C)c1ccc(C(C)(C)C(C)(C)c2ccc(C(C)(C)C)cc2)cc1
Mol. weight [g/mol]: 350.58
CAS: 5171-91-5

Physical Properties

Property code	Value	Unit	Source
chs	-15360.70 ± 2.70	kJ/mol	NIST Webbook
gf	384.96	kJ/mol	Joback Method
hf	-139.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-301.30 ± 2.70	kJ/mol	NIST Webbook
hfus	20.74	kJ/mol	Joback Method
hsub	162.30	kJ/mol	NIST Webbook
hvap	74.16	kJ/mol	Joback Method
log10ws	-7.54		Crippen Method
logp	7.537		Crippen Method
mcvol	329.680	ml/mol	McGowan Method
pc	1106.68	kPa	Joback Method
tb	844.68	K	Joback Method
tc	1082.95	K	Joback Method
tf	470.34	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1045.55	J/mol×K	844.68	Joback Method
cpg	1067.32	J/mol×K	884.39	Joback Method
cpg	1087.67	J/mol×K	924.10	Joback Method
cpg	1106.83	J/mol×K	963.81	Joback Method
cpg	1125.01	J/mol×K	1003.53	Joback Method
cpg	1142.44	J/mol×K	1043.24	Joback Method

cpg	1159.34	J/mol×K	1082.95	Joback Method
cps	529.50	J/mol×K	298.00	NIST Webbook
dvisc	0.0005888	Pa×s	470.34	Joback Method
dvisc	0.0002352	Pa×s	532.73	Joback Method
dvisc	0.0001139	Pa×s	595.12	Joback Method
dvisc	0.0000633	Pa×s	657.51	Joback Method
dvisc	0.0000389	Pa×s	719.90	Joback Method
dvisc	0.0000259	Pa×s	782.29	Joback Method
dvisc	0.0000183	Pa×s	844.68	Joback Method
hfust	43.93	kJ/mol	493.00	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=C5171915&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume

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