2,4-Bis(dimethylbenzyl)-6-t-butylphenol

Other names: 2-(Tert-butyl)-4,6-bis(2-phenylpropan-2-yl)phenol
Inchi: InChI=1S/C28H34O/c1-26(2,3)23-18-22(27(4,5)20-14-10-8-11-15-20)19-24(25(23)29)28(
InchiKey: QIJHCZVVJYQNJA-UHFFFAOYSA-N
Formula: C28H34O
SMILES: CC(C)(C)c1cc(C(C)(C)c2ccccc2)cc(C(C)(C)c2ccccc2)c1O
Mol. weight [g/mol]: 386.57
CAS: 244080-16-8

Physical Properties

Property code	Value	Unit	Source
gf	356.75	kJ/mol	Joback Method
hf	-138.16	kJ/mol	Joback Method
hfus	33.16	kJ/mol	Joback Method
hvap	95.20	kJ/mol	Joback Method
log10ws	-7.56		Crippen Method
logp	7.341		Crippen Method
mcvol	339.970	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
rinpol	2547.30		NIST Webbook
rinpol	2547.30		NIST Webbook
tb	1000.97	K	Joback Method
tc	1262.85	K	Joback Method
tf	628.60	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.50	J/mol×K	1000.97	Joback Method
cpg	1149.86	J/mol×K	1044.62	Joback Method
cpg	1170.05	J/mol×K	1088.26	Joback Method
cpg	1190.42	J/mol×K	1131.91	Joback Method
cpg	1211.31	J/mol×K	1175.56	Joback Method
cpg	1233.08	J/mol×K	1219.21	Joback Method

cpg	1256.06	J/mol×K	1262.85	Joback Method
dvisc	0.0000205	Pa×s	628.60	Joback Method
dvisc	0.0000085	Pa×s	690.66	Joback Method
dvisc	0.0000041	Pa×s	752.72	Joback Method
dvisc	0.0000022	Pa×s	814.79	Joback Method
dvisc	0.0000013	Pa×s	876.85	Joback Method
dvisc	0.0000008	Pa×s	938.91	Joback Method
dvisc	0.0000005	Pa×s	1000.97	Joback Method

Sources

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=C244080168&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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