2,6-BIS(t-BUTYL)-4-(DIMETHYLBENZYL)PHENOL

Other names: 2,6-Bis(t-butyl)-4-(dimethylbenzyl)phenol
2,6-bis(tert-butyl)-4-(1-methyl-1-phenylethyl)phenol
2,6-Di-tert-butyl-4-(2-phenylpropan-2-yl)phenol
Inchi: InChI=1S/C23H32O/c1-21(2,3)18-14-17(15-19(20(18)24)22(4,5)6)23(7,8)16-12-10-9-11-
InchiKey: ROEHFIIRMUXFRR-UHFFFAOYSA-N
Formula: C23H32O
SMILES: CC(C)(C)c1cc(C(C)(C)c2ccccc2)cc(C(C)(C)C)c1O
Mol. weight [g/mol]: 324.51

Physical Properties

Property code	Value	Unit	Source
af	0.7224		Cheméo Relay (1.0)
hf	-227.12	kJ/mol	Cheméo Relay (1.0)
hfus	26.17	kJ/mol	Joback Method
hvap	108.36	kJ/mol	Cheméo Relay (1.0)
ie	7.70	eV	Cheméo Relay (1.0)
log10ws	-6.55		Cheméo Relay (1.0)
logp	6.313		Crippen Method
mcvol	293.280	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
rinpol	2083.20		NIST Webbook
rinpol	2083.20		NIST Webbook
tb	598.64	K	Cheméo Relay (1.0)
tc	905.92	K	Cheméo Relay (1.0)
tf	385.73	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	926.37	J/mol×K	859.89	Joback Method
cpg	945.78	J/mol×K	900.76	Joback Method
cpg	964.27	J/mol×K	941.62	Joback Method
cpg	982.11	J/mol×K	982.49	Joback Method
cpg	999.54	J/mol×K	1023.36	Joback Method

cpg	1016.81	J/mol×K	1064.23	Joback Method
cpg	1034.17	J/mol×K	1105.09	Joback Method
dvisc	0.0000732	Pa×s	545.83	Joback Method
dvisc	0.0000295	Pa×s	598.17	Joback Method
dvisc	0.0000137	Pa×s	650.52	Joback Method
dvisc	0.0000072	Pa×s	702.86	Joback Method
dvisc	0.0000041	Pa×s	755.20	Joback Method
dvisc	0.0000025	Pa×s	807.55	Joback Method
dvisc	0.0000016	Pa×s	859.89	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C34624812&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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