2-TERT-BUTYL-4-METHYL-6-(A-METHYLBENZYL)

Other names: 2-tert-butyl-4-methyl-6-«alpha»-methylbenzylphenol
Inchi: InChI=1S/C19H24O/c1-13-11-16(14(2)15-9-7-6-8-10-15)18(20)17(12-13)19(3,4)5/h6-12,
InchiKey: KYWXWCOPNNMDMN-UHFFFAOYSA-N
Formula: C19H24O
SMILES: Cc1cc(C(C)c2ccccc2)c(O)c(C(C)(C)C)c1
Mol. weight [g/mol]: 268.40

Physical Properties

Property code	Value	Unit	Source
hf	-140.09	kJ/mol	Cheméo Relay (1.0)
hfus	27.12	kJ/mol	Joback Method
hvap	106.56	kJ/mol	Cheméo Relay (1.0)
ie	7.66	eV	Cheméo Relay (1.0)
logp	5.150		Crippen Method
mcvol	236.920	ml/mol	McGowan Method
tb	594.76	K	Cheméo Relay (1.0)
tf	338.00 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	772.92	J/mol×K	976.94	Joback Method
cpg	786.77	J/mol×K	1017.45	Joback Method
cpg	711.33	J/mol×K	814.90	Joback Method
cpg	727.99	J/mol×K	855.41	Joback Method
cpg	743.69	J/mol×K	895.92	Joback Method
cpg	758.61	J/mol×K	936.43	Joback Method
cpg	693.55	J/mol×K	774.39	Joback Method
dvisc	0.0000459	Pa×s	578.74	Joback Method
dvisc	0.0000995	Pa×s	529.82	Joback Method
dvisc	0.0002527	Pa×s	480.91	Joback Method
dvisc	0.0000239	Pa×s	627.65	Joback Method
dvisc	0.0000136	Pa×s	676.56	Joback Method
dvisc	0.0000084	Pa×s	725.48	Joback Method

dvisc	0.0000055	Pa×s	774.39	Joback Method
hfust	31.38	kJ/mol	337.70	NIST Webbook

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1706656&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point