

(5-Tert-butyl-2-hydroxyphenyl)(4-chlorophenyl)methane

Inchi:	InChI=1S/C17H17ClO2/c1-17(2,3)12-6-9-15(19)14(10-12)16(20)11-4-7-13(18)8-5-11/h4-
InchiKey:	HMWLCGKWJDGQSS-UHFFFAOYSA-N
Formula:	C17H17ClO2
SMILES:	CC(C)(C)c1ccc(O)c(C(=O)c2ccc(Cl)cc2)c1
Mol. weight [g/mol]:	288.77
CAS:	72083-19-3

Physical Properties

Property code	Value	Unit	Source
gf	5.19	kJ/mol	Joback Method
hf	-258.47	kJ/mol	Joback Method
hfus	31.26	kJ/mol	Joback Method
hvap	82.16	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.574		Crippen Method
mcvol	222.550	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
tb	820.37	K	Joback Method
tc	1075.28	K	Joback Method
tf	553.22	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.60	J/molxK	820.37	Joback Method
cpg	634.46	J/molxK	862.86	Joback Method
cpg	647.48	J/molxK	905.34	Joback Method
cpg	659.85	J/molxK	947.83	Joback Method
cpg	671.75	J/molxK	990.31	Joback Method
cpg	683.37	J/molxK	1032.80	Joback Method
cpg	694.89	J/molxK	1075.28	Joback Method
dvisc	0.0001120	Paxs	553.22	Joback Method
dvisc	0.0000568	Paxs	597.75	Joback Method

dvisc	0.0000316	Paxs	642.27	Joback Method
dvisc	0.0000190	Paxs	686.80	Joback Method
dvisc	0.0000122	Paxs	731.32	Joback Method
dvisc	0.0000082	Paxs	775.85	Joback Method
dvisc	0.0000057	Paxs	820.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72083193&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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