

(5-Tert-butyl-2-hydroxyphenyl)(phenyl)methanone

Inchi:	InChI=1S/C17H18O2/c1-17(2,3)13-9-10-15(18)14(11-13)16(19)12-7-5-4-6-8-12/h4-11,18
InchiKey:	IAAWULFRQOKLJI-UHFFFAOYSA-N
Formula:	C17H18O2
SMILES:	CC(C)(C)c1ccc(O)c(C(=O)c2ccccc2)c1
Mol. weight [g/mol]:	254.32
CAS:	10425-05-5

Physical Properties

Property code	Value	Unit	Source
gf	26.75	kJ/mol	Joback Method
hf	-231.26	kJ/mol	Joback Method
hfus	27.45	kJ/mol	Joback Method
hvap	77.11	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.921		Crippen Method
mcvol	210.310	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
tb	777.96	K	Joback Method
tc	1030.47	K	Joback Method
tf	510.78	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.83	J/molxK	777.96	Joback Method
cpg	613.92	J/molxK	820.05	Joback Method
cpg	627.99	J/molxK	862.13	Joback Method
cpg	641.23	J/molxK	904.22	Joback Method
cpg	653.80	J/molxK	946.30	Joback Method
cpg	665.91	J/molxK	988.39	Joback Method
cpg	677.73	J/molxK	1030.47	Joback Method
dvisc	0.0002033	Paxs	510.78	Joback Method
dvisc	0.0000938	Paxs	555.31	Joback Method

dvisc	0.0000486	Paxs	599.84	Joback Method
dvisc	0.0000275	Paxs	644.37	Joback Method
dvisc	0.0000168	Paxs	688.90	Joback Method
dvisc	0.0000109	Paxs	733.43	Joback Method
dvisc	0.0000074	Paxs	777.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10425055&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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