2,2-Dimethyl-1-phenyl-1-propanol

Other names: Benzenemethanol, «alpha»-(1,1-dimethylethyl)-
1-Phenyl-2,2-dimethyl-1-propanol
tert-Butylphenylmethanol
Inchi: InChI=1S/C11H16O/c1-11(2,3)10(12)9-7-5-4-6-8-9/h4-8,10,12H,1-3H3
InchiKey: YBVRFTBNIZWMSK-UHFFFAOYSA-N
Formula: C11H16O
SMILES: CC(C)(C)C(O)c1ccccc1
Mol. weight [g/mol]: 164.24
CAS: 3835-64-1

Physical Properties

Property code	Value	Unit	Source
gf	17.73	kJ/mol	Joback Method
hf	-200.10	kJ/mol	Joback Method
hfus	11.44	kJ/mol	Joback Method
hvap	57.35	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.766		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
tb	566.27	K	Joback Method
tc	771.45	K	Joback Method
tf	318.00 ± 2.00	K	NIST Webbook
tf	323.65 ± 2.00	K	NIST Webbook
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.20	J/mol×K	566.27	Joback Method
cpg	376.58	J/mol×K	600.47	Joback Method
cpg	390.01	J/mol×K	634.66	Joback Method
cpg	402.55	J/mol×K	668.86	Joback Method
cpg	414.26	J/mol×K	703.06	Joback Method

cpg	425.19	J/mol×K	737.25	Joback Method
cpg	435.39	J/mol×K	771.45	Joback Method
dvisc	0.0245558	Pa×s	288.39	Joback Method
dvisc	0.0048567	Pa×s	334.70	Joback Method
dvisc	0.0014244	Pa×s	381.02	Joback Method
dvisc	0.0005450	Pa×s	427.33	Joback Method
dvisc	0.0002516	Pa×s	473.64	Joback Method
dvisc	0.0001333	Pa×s	519.96	Joback Method
dvisc	0.0000784	Pa×s	566.27	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	363.20	K	0.70	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3835641&Units=SI

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume