2-Methyl-1-phenyl-2-propanol

Other names:	Phenethyl alcohol, «alpha»,«alpha»-dimethyl- «alpha»,«alpha»-Dimethylphenethanol «alpha»,«alpha»-Dimethylphenethyl alcohol Benzyldimethylcarbinol Dimethylbenzylcarbinol DMBC 1,1-Dimethyl-2-Phenylethanol 1,1-Dimethylphenylethanol 2-Methyl-1-phenyl-2-propanol Phenyl-tert-butanol «alpha»,«alpha»-Dimethyl-«beta»-phenylethyl alcohol «beta»-Phenyl-tert-butyl alcohol 2-Benzyl-2-propanol 2-Hydroxy-2-methyl-1-phenylpropane 2-Methyl-3-phenyl-2-propanol 1,1-Dimethyl-2-phenylethyl alcohol 2-Methyl-1-phenylpropan-2-ol Ethanol, 1,1-dimethyl-2-phenyl- «alpha»,«alpha»-Dimethylphenylethyl alcohol NSC 27228
Inchi:	InChI=1S/C10H14O/c1-10(2,11)8-9-6-4-3-5-7-9/h3-7,11H,8H2,1-2H3
InchiKey:	RIWRBSMFKVOJMN-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CC(C)(O)Cc1ccccc1
Mol. weight [g/mol]:	150.22

Physical Properties

Property code	Value	Unit	Source
af	0.6216		Cheméo Relay (1.0)
gf	11.75	kJ/mol	Joback Method
hf	-211.41	kJ/mol	Cheméo Relay (1.0)
hfus	12.37	kJ/mol	Joback Method
hvap	68.65	kJ/mol	Cheméo Relay (1.0)
ie	8.89	eV	Cheméo Relay (1.0)
log10ws	-1.21		Cheméo Relay (1.0)
logp	2.000		Crippen Method
mcvol	133.870	ml/mol	McGowan Method

pc	3318.18	kPa	Joback Method
rinpol	1124.60		NIST Webbook
rinpol	1140.90		NIST Webbook
rinpol	1126.70		NIST Webbook
rinpol	1124.60		NIST Webbook
ripol	1753.90		NIST Webbook
ripol	1751.40		NIST Webbook
ripol	1781.00		NIST Webbook
ripol	1781.00		NIST Webbook
tb	488.20	K	NIST Webbook
tc	709.08	K	Cheméo Relay (1.0)
tf	323.41	K	Cheméo Relay (1.0)
vc	0.493	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.14	J/mol×K	543.83	Joback Method
cpg	328.48	J/mol×K	577.83	Joback Method
cpg	340.94	J/mol×K	611.82	Joback Method
cpg	352.57	J/mol×K	645.82	Joback Method
cpg	363.42	J/mol×K	679.82	Joback Method
cpg	373.54	J/mol×K	713.82	Joback Method
cpg	382.98	J/mol×K	747.81	Joback Method
dvisc	0.0171729	Pa×s	292.12	Joback Method
dvisc	0.0042551	Pa×s	334.07	Joback Method
dvisc	0.0014394	Pa×s	376.02	Joback Method
dvisc	0.0006053	Pa×s	417.97	Joback Method
dvisc	0.0002981	Pa×s	459.93	Joback Method
dvisc	0.0001653	Pa×s	501.88	Joback Method
dvisc	0.0001003	Pa×s	543.83	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.20	K	1.30	NIST Webbook

Sources

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=C100867&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume