Benzeneethanol, 2-methyl-

Other names:	o-Methylphenethyl alcohol
	2-Methylphenethyl alcohol
	Phenethyl alcohol, o-methyl-
	2-(2-Methylphenyl)ethanol
	Phenethyl alcohol, 2'-methyl
	2-o-tolylethanol
Inchi:	InChI=1S/C9H12O/c1-8-4-2-3-5-9(8)6-7-10/h2-5,10H,6-7H2,1H3
InchiKey:	RUGISKODRCWQNE-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	Cc1ccccc1CCO
Mol. weight [g/mol]:	136.19
CAS:	19819-98-8

Physical Properties

Property code	Value	Unit	Source
gf	-9.14	kJ/mol	Joback Method
hf	-156.26	kJ/mol	Joback Method
hfus	16.81	kJ/mol	Joback Method
hvap	55.25	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.530		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
rinpol	1216.00		NIST Webbook
rinpol	1216.00		NIST Webbook
ripol	2012.00		NIST Webbook
tb	516.70	K	NIST Webbook
tc	725.15	K	Joback Method
tf	290.95	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	266.45	J/mol×K	529.16	Joback Method
cpg	277.78	J/mol×K	561.83	Joback Method
cpg	288.52	J/mol×K	594.49	Joback Method
cpg	298.68	J/mol×K	627.16	Joback Method
cpg	308.29	J/mol×K	659.82	Joback Method
cpg	317.36	J/mol×K	692.49	Joback Method
cpg	325.92	J/mol×K	725.15	Joback Method
dvisc	0.0098792	Pa×s	290.95	Joback Method
dvisc	0.0030353	Pa×s	330.65	Joback Method
dvisc	0.0012010	Pa×s	370.35	Joback Method
dvisc	0.0005687	Pa×s	410.05	Joback Method
dvisc	0.0003073	Pa×s	449.76	Joback Method
dvisc	0.0001835	Pa×s	489.46	Joback Method
dvisc	0.0001184	Pa×s	529.16	Joback Method

Sources

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=C19819988&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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

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