BENZENETHANOL, alpha-METHYL-

Other names:	.alpha.-methylphenethyl alcohol
	1-phenyl-2-propanol
	1-phenylpropan-2-ol
	2-Hydroxy-1-phenylpropane
	2-propanol, 1-phenyl-
	Benzenethanol, «alpha»-methyl-
	Benzyl methyl carbinol
	NSC 53553
	Phenethyl alcohol, «alpha»-methyl-
	benzylmethylcarbinol
	«alpha»-Methylbenzeneethanol
	«alpha»-Methylphenethyl alcohol
Inchi:	InChI=1S/C9H12O/c1-8(10)7-9-5-3-2-4-6-9/h2-6,8,10H,7H2,1H3
InchiKey:	WYTRYIUQUDTGSX-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	CC(O)Cc1ccccc1
Mol. weight [g/mol]:	136.19

Physical Properties

Property code	Value	Unit	Source
af	0.5841		Cheméo Relay (1.0)
gf	-1.95	kJ/mol	Joback Method
hf	-175.59	kJ/mol	Cheméo Relay (1.0)
hfus	13.67	kJ/mol	Joback Method
hvap	69.92	kJ/mol	Cheméo Relay (1.0)
ie	8.93	eV	Cheméo Relay (1.0)
log10ws	-0.85		Cheméo Relay (1.0)
logp	1.610		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
rinpol	1212.00		NIST Webbook
rinpol	1212.00		NIST Webbook
ripol	1771.00		NIST Webbook
ripol	1779.00		NIST Webbook
ripol	1778.00		NIST Webbook
ripol	1773.00		NIST Webbook
ripol	1771.00		NIST Webbook

tb	498.95	K	Cheméo Relay (1.0)
tc	695.35	K	Cheméo Relay (1.0)
tf	270.65	K	Cheméo Relay (1.0)
vc	0.440	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.28	J/mol×K	590.10	Joback Method
cpg	329.13	J/mol×K	722.83	Joback Method
cpg	320.31	J/mol×K	689.65	Joback Method
cpg	310.91	J/mol×K	656.46	Joback Method
cpg	300.91	J/mol×K	623.28	Joback Method
cpg	267.01	J/mol×K	523.74	Joback Method
cpg	278.99	J/mol×K	556.92	Joback Method
cpl	354.78	J/mol×K	473.15	Melting Point, Enthalpy of Fusion, and Heat Capacity Measurements of Several Polyfunctional, Industrially Important Compounds by Differential Scanning Calorimetry
cpl	282.05	J/mol×K	273.15	Melting Point, Enthalpy of Fusion, and Heat Capacity Measurements of Several Polyfunctional, Industrially Important Compounds by Differential Scanning Calorimetry

cpl	345.52	J/mol×K	423.15	Melting Point, Enthalpy of Fusion, and Heat Capacity Measurements of Several Polyfunctional, Industrially Important Compounds by Differential Scanning Calorimetry
cpl	329.31	J/mol×K	373.15	Melting Point, Enthalpy of Fusion, and Heat Capacity Measurements of Several Polyfunctional, Industrially Important Compounds by Differential Scanning Calorimetry
cpl	311.06	J/mol×K	323.15	Melting Point, Enthalpy of Fusion, and Heat Capacity Measurements of Several Polyfunctional, Industrially Important Compounds by Differential Scanning Calorimetry
dvisc	0.0307952	Pa×s	263.43	Joback Method
dvisc	0.0063252	Pa×s	306.81	Joback Method
dvisc	0.0019230	Pa×s	350.20	Joback Method
dvisc	0.0007602	Pa×s	393.59	Joback Method
dvisc	0.0003613	Pa×s	436.97	Joback Method
dvisc	0.0001964	Pa×s	480.36	Joback Method
dvisc	0.0001181	Pa×s	523.74	Joback Method

Sources

Cheméo Relay (1.0, beta):

Melting Point, Enthalpy of Fusion, and Heat Capacity Measurements of Several Polyfunctional, Industrially Important Compounds by Differential Scanning Calorimetry: https://www.doi.org/10.1021/acs.jced.7b01026

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C698873&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume