.alpha.-Methylbenzenepropanol

Other names: 2-Methyl-3-phenyl-1-propanol
2-methyl-3-phenylpropanol
Inchi: InChI=1S/C10H14O/c1-9(8-11)7-10-5-3-2-4-6-10/h2-6,9,11H,7-8H2,1H3
InchiKey: LTZKHYYXQWNXPU-UHFFFAOYSA-N
Formula: C10H14O
SMILES: CC(CO)Cc1ccccc1
Mol. weight [g/mol]: 150.22

Physical Properties

Property code	Value	Unit	Source
af	0.6243		Cheméo Relay (1.0)
gf	6.47	kJ/mol	Joback Method
hf	-170.56	kJ/mol	Cheméo Relay (1.0)
hfus	16.26	kJ/mol	Joback Method
hvap	78.83	kJ/mol	Cheméo Relay (1.0)
ie	8.74	eV	Cheméo Relay (1.0)
log10ws	-1.57		Cheméo Relay (1.0)
logp	1.857		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
tb	519.28	K	Cheméo Relay (1.0)
tc	727.17	K	Cheméo Relay (1.0)
tf	250.47	K	Cheméo Relay (1.0)
vc	0.467	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.06	J/mol×K	546.62	Joback Method
cpg	324.88	J/mol×K	579.35	Joback Method
cpg	336.98	J/mol×K	612.08	Joback Method
cpg	348.39	J/mol×K	644.81	Joback Method
cpg	359.13	J/mol×K	677.54	Joback Method
cpg	369.24	J/mol×K	710.27	Joback Method

cpg	378.75	J/mol×K	743.00	Joback Method
dvisc	0.0247773	Pa×s	274.70	Joback Method
dvisc	0.0051616	Pa×s	320.02	Joback Method
dvisc	0.0015868	Pa×s	365.34	Joback Method
dvisc	0.0006329	Pa×s	410.66	Joback Method
dvisc	0.0003030	Pa×s	455.98	Joback Method
dvisc	0.0001658	Pa×s	501.30	Joback Method
dvisc	0.0001002	Pa×s	546.62	Joback Method
hvapt	71.90	kJ/mol	368.00	NIST Webbook

Sources

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):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7384807&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
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