2,3-Butanediol, 2,3-diphenyl-

Other names:	Acetophenonepinacol
	1,2-Dimethyl-1,2-diphenylethylene glycol
	2,3-Dihydroxy-2,3-diphenylbutane
	2,3-Diphenyl-2,3-butanediol
	2,3-Diphenyl-2,3-dihydroxybutane
	2,3-diphenylbutane-2,3-diol
Inchi:	InChI=1S/C16H18O2/c1-15(17,13-9-5-3-6-10-13)16(2,18)14-11-7-4-8-12-14/h3-12,17-18
InchiKey:	URPRLFISKOCZHR-UHFFFAOYSA-N
Formula:	C16H18O2
SMILES:	CC(O)(c1ccccc1)C(C)(O)c1ccccc1
Mol. weight [g/mol]:	242.31
CAS:	1636-34-6

Physical Properties

Property code	Value	Unit	Source
gf	40.70	kJ/mol	Joback Method
hf	-222.47	kJ/mol	Joback Method
hfus	18.63	kJ/mol	Joback Method
hvap	86.53	kJ/mol	Joback Method
ie	9.01 ± 0.02	eV	NIST Webbook
log10ws	-3.59		Crippen Method
logp	2.802		Crippen Method
mcvol	200.520	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
tb	796.74	K	Joback Method
tc	1016.71	K	Joback Method
tf	449.40	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.52	J/mol×K	796.74	Joback Method
cpg	602.59	J/mol×K	833.40	Joback Method

cpg	613.77	J/mol×K	870.06	Joback Method
cpg	624.18	J/mol×K	906.72	Joback Method
cpg	633.95	J/mol×K	943.39	Joback Method
cpg	643.17	J/mol×K	980.05	Joback Method
cpg	651.98	J/mol×K	1016.71	Joback Method
dvisc	0.0009775	Pa×s	449.40	Joback Method
dvisc	0.0002239	Pa×s	507.29	Joback Method
dvisc	0.0000694	Pa×s	565.18	Joback Method
dvisc	0.0000267	Pa×s	623.07	Joback Method
dvisc	0.0000121	Pa×s	680.96	Joback Method
dvisc	0.0000062	Pa×s	738.85	Joback Method
dvisc	0.0000035	Pa×s	796.74	Joback Method

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=C1636346&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
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

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