Benzeneethanol, «alpha»-(2-methylpropyl)-

Other names: iso-Butyl benzyl carbinol
2-Pentanol, 4-methyl-1-phenyl
4-methyl-1-phenylpentan-2-ol
Inchi: InChI=1S/C12H18O/c1-10(2)8-12(13)9-11-6-4-3-5-7-11/h3-7,10,12-13H,8-9H2,1-2H3
InchiKey: IUADYGVMSDKSMB-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CC(C)CC(O)Cc1ccccc1
Mol. weight [g/mol]: 178.27
CAS: 7779-78-4

Physical Properties

Property code	Value	Unit	Source
gf	20.87	kJ/mol	Joback Method
hf	-217.27	kJ/mol	Joback Method
hfus	17.92	kJ/mol	Joback Method
hvap	60.48	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.636		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
rinpol	1366.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1366.00		NIST Webbook
ripol	1983.00		NIST Webbook
tb	591.94	K	Joback Method
tc	787.01	K	Joback Method
tf	282.24	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.68	J/mol×K	591.94	Joback Method
cpg	422.21	J/mol×K	624.45	Joback Method

cpg	435.93	J/mol×K	656.96	Joback Method
cpg	448.87	J/mol×K	689.48	Joback Method
cpg	461.06	J/mol×K	721.99	Joback Method
cpg	472.53	J/mol×K	754.50	Joback Method
cpg	483.32	J/mol×K	787.01	Joback Method
dvisc	0.0286301	Pa×s	282.24	Joback Method
dvisc	0.0047767	Pa×s	333.86	Joback Method
dvisc	0.0012874	Pa×s	385.47	Joback Method
dvisc	0.0004729	Pa×s	437.09	Joback Method
dvisc	0.0002146	Pa×s	488.71	Joback Method
dvisc	0.0001133	Pa×s	540.32	Joback Method
dvisc	0.0000668	Pa×s	591.94	Joback Method

Sources

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=C7779784&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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