

3-Buten-2-ol, 4-phenyl-

Other names:	«alpha»-Methyl-«gamma»-phenylallyl alcohol 1-Methyl-3-phenylallyl alcohol 4-Phenyl-3-buten-2-ol «alpha»-Methyl-3-phenylallyl alcohol
Inchi:	InChI=1S/C10H12O/c1-9(11)7-8-10-5-3-2-4-6-10/h2-9,11H,1H3/b8-7+
InchiKey:	ZIJWGEHOVHJHKB-BQYQJAHWSA-N
Formula:	C10H12O
SMILES:	CC(O)C=Cc1ccccc1
Mol. weight [g/mol]:	148.20
CAS:	17488-65-2

Physical Properties

Property code	Value	Unit	Source
gf	86.69	kJ/mol	Joback Method
hf	-53.49	kJ/mol	Joback Method
hfus	16.46	kJ/mol	Joback Method
hvap	56.38	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.081		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpol	1329.00		NIST Webbook
tb	550.78	K	Joback Method
tc	755.82	K	Joback Method
tf	269.62	K	Joback Method
vc	0.480	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.06	J/mol×K	550.78	Joback Method
cpg	347.04	J/mol×K	721.65	Joback Method
cpg	337.63	J/mol×K	687.48	Joback Method
cpg	327.57	J/mol×K	653.30	Joback Method

cpg	316.82	J/mol×K	619.13	Joback Method
cpg	305.33	J/mol×K	584.95	Joback Method
cpg	355.85	J/mol×K	755.82	Joback Method
dvisc	0.0000833	Paxs	550.78	Joback Method
dvisc	0.0001387	Paxs	503.92	Joback Method
dvisc	0.0002564	Paxs	457.06	Joback Method
dvisc	0.0005452	Paxs	410.20	Joback Method
dvisc	0.0014087	Paxs	363.34	Joback Method
dvisc	0.0048211	Paxs	316.48	Joback Method
dvisc	0.0253050	Paxs	269.62	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=C17488652&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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