2-Methyl-3-phenyl-2-propen-1-ol

Other names: 2-Propen-1-ol, 2-methyl-3-phenyl-
Cinnamyl alcohol, «alpha»-methyl-
Methyl cinnamic alcohol
«alpha»-Methylcinnamyl alcohol
3-Phenyl-2-methyl-propen-2-ol-1
1-Phenyl-2-methylprop-1-ene-3-ol
«alpha»-Methylcinnamic alcohol
«beta»-methylcinnamyl alcohol

Inchi: InChI=1S/C10H12O/c1-9(8-11)7-10-5-3-2-4-6-10/h2-7,11H,8H2,1H3/b9-7-

InchiKey: LLNAMUJRIZIXHF-CLFYSBASSA-N

Formula: C10H12O

SMILES: CC(=Cc1ccccc1)CO

Mol. weight [g/mol]: 148.20

CAS: 1504-55-8

Physical Properties

Property code	Value	Unit	Source
gf	80.58	kJ/mol	Joback Method
hf	-58.00	kJ/mol	Joback Method
hfus	18.68	kJ/mol	Joback Method
hvap	56.85	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.082		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinpol	1343.00		NIST Webbook
rinpol	1343.00		NIST Webbook
ripol	2252.00		NIST Webbook
ripol	2252.00		NIST Webbook
tb	551.10	K	Joback Method
tc	755.46	K	Joback Method
tf	270.66	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.52	J/mol×K	551.10	Joback Method
cpg	304.65	J/mol×K	585.16	Joback Method
cpg	316.02	J/mol×K	619.22	Joback Method
cpg	326.66	J/mol×K	653.28	Joback Method
cpg	336.63	J/mol×K	687.34	Joback Method
cpg	345.97	J/mol×K	721.40	Joback Method
cpg	354.73	J/mol×K	755.46	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1504558&Units=SI
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

Legend

cpg: Ideal gas heat capacity
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