2-Benzylidene-1-heptanol

Other names:	1-Heptanol, 2-(phenylmethylene)-
	1-Heptanol, 2-benzylidene-
	«alpha»-Amylcinnamic alcohol
	«alpha»-Amylcinnamyl alcohol
	2-Amyl-3-phenyl-2-propen-1-ol
	Buxinol
	2-Pentyl-3-phenyl-2-propen-1-ol
	Amyl cinnamyl alcohol
	Amyl cinnamic alcohol
	2-pentyl-3-phenylprop-2-en-1-ol
Inchi:	InChI=1S/C14H20O/c1-2-3-5-10-14(12-15)11-13-8-6-4-7-9-13/h4,6-9,11,15H,2-3,5,10,12
InchiKey:	LIPHCKNQPJXUQF-SDNWHVSQSA-N
Formula:	C14H20O
SMILES:	CCCCCC(=Cc1ccccc1)CO
Mol. weight [g/mol]:	204.31
CAS:	101-85-9

Physical Properties

Property code	Value	Unit	Source
gf	114.26	kJ/mol	Joback Method
hf	-140.56	kJ/mol	Joback Method
hfus	29.04	kJ/mol	Joback Method
hvap	65.75	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.643		Crippen Method
mcvol	185.930	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
rinpol	1675.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1684.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1677.00		NIST Webbook
tb	642.62	K	Joback Method

tc	836.25	K	Joback Method
tf	315.74	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.74	J/mol×K	642.62	Joback Method
cpg	501.41	J/mol×K	674.89	Joback Method
cpg	515.24	J/mol×K	707.16	Joback Method
cpg	528.29	J/mol×K	739.44	Joback Method
cpg	540.61	J/mol×K	771.71	Joback Method
cpg	552.24	J/mol×K	803.98	Joback Method
cpg	563.23	J/mol×K	836.25	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=C101859&Units=SI

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

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume