BENZENEACETALDEHYDE, .ALPHA.-(2-METHYLPROPYLIDENE)-

Other names: 4-Methyl-2-phenyl-2-pentenal
2-Pentenal, 4-methyl-2-phenyl
Inchi: InChI=1S/C12H14O/c1-10(2)8-12(9-13)11-6-4-3-5-7-11/h3-10H,1-2H3/b12-8+
InchiKey: ULRYRAHIBWLZKC-XYOKQWHBSA-N
Formula: C12H14O
SMILES: CC(C)/C=C(\C=O)c1ccccc1
Mol. weight [g/mol]: 174.24

Physical Properties

Property code	Value	Unit	Source
hfus	18.54	kJ/mol	Joback Method
logp	2.925		Crippen Method
mcvol	153.450	ml/mol	McGowan Method
rinpol	1383.00		NIST Webbook
ripol	1932.00		NIST Webbook
ripol	1920.00		NIST Webbook
ripol	1920.00		NIST Webbook
tb	514.26	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.34	J/mol×K	552.90	Joback Method
cpg	365.68	J/mol×K	589.75	Joback Method
cpg	379.99	J/mol×K	626.60	Joback Method
cpg	393.32	J/mol×K	663.45	Joback Method
cpg	405.73	J/mol×K	700.30	Joback Method
cpg	417.29	J/mol×K	737.15	Joback Method
cpg	428.05	J/mol×K	774.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26643914&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature