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
CAS: 26643-91-4

Physical Properties

Property code	Value	Unit	Source
gf	132.28	kJ/mol	Joback Method
hf	-37.91	kJ/mol	Joback Method
hfus	18.54	kJ/mol	Joback Method
hvap	50.95	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.925		Crippen Method
mcvol	153.450	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
rinpol	1383.00		NIST Webbook
ripol	1920.00		NIST Webbook
ripol	1920.00		NIST Webbook
ripol	1932.00		NIST Webbook
tb	552.90	K	Joback Method
tc	774.00	K	Joback Method
tf	259.38	K	Joback Method
vc	0.592	m3/kmol	Joback Method

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

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=C26643914&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume