5-Methyl-2-phenyl-2-hexenal

Other names: Benzeneacetaldehyde, «alpha»-(3-methylbutylidene)-
2-Phenyl-5-methyl-2-hexenal
2-Phenyl-5-methylhex-2-enal
5-methyl-2-phenylhex-2-enal
Inchi: InChI=1S/C13H16O/c1-11(2)8-9-13(10-14)12-6-4-3-5-7-12/h3-7,9-11H,8H2,1-2H3/b13-9
InchiKey: YURDCJXYOLERLO-LCYFTJDESA-N
Formula: C13H16O
SMILES: CC(C)CC=C(C=O)c1ccccc1
Mol. weight [g/mol]: 188.27
CAS: 21834-92-4

Physical Properties

Property code	Value	Unit	Source
gf	140.70	kJ/mol	Joback Method
hf	-58.55	kJ/mol	Joback Method
hfus	21.13	kJ/mol	Joback Method
hvap	53.18	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.315		Crippen Method
mcvol	167.540	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	1486.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1485.00		NIST Webbook
ripol	2052.00		NIST Webbook
ripol	2024.00		NIST Webbook
ripol	2083.00		NIST Webbook
ripol	2060.00		NIST Webbook

tb	575.78	K	Joback Method
tc	792.99	K	Joback Method
tf	270.65	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.02	J/mol×K	575.78	Joback Method
cpg	414.02	J/mol×K	611.98	Joback Method
cpg	428.96	J/mol×K	648.18	Joback Method
cpg	442.92	J/mol×K	684.39	Joback Method
cpg	455.95	J/mol×K	720.59	Joback Method
cpg	468.11	J/mol×K	756.79	Joback Method
cpg	479.46	J/mol×K	792.99	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=C21834924&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