1-Nonen-3-one, 1-phenyl-

Other names: «alpha»-n-Hexyl cinnamic aldehyde
Inchi: InChI=1S/C15H20O/c1-2-3-4-8-11-15(16)13-12-14-9-6-5-7-10-14/h5-7,9-10,12-13H,2-4,8
InchiKey: NUWFGSCHUJWGHJ-OUKQBFOZSA-N
Formula: C15H20O
SMILES: CCCCCCC(=O)C=Cc1ccccc1
Mol. weight [g/mol]: 216.32
CAS: 30669-47-7

Physical Properties

Property code	Value	Unit	Source
gf	139.13	kJ/mol	Joback Method
hf	-111.76	kJ/mol	Joback Method
hfus	30.45	kJ/mol	Joback Method
hvap	57.96	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.239		Crippen Method
mcvol	195.720	ml/mol	McGowan Method
pc	2043.76	kPa	Joback Method
rinpol	1727.00		NIST Webbook
rinpol	1727.00		NIST Webbook
ripol	2309.00		NIST Webbook
tb	627.31	K	Joback Method
tc	834.32	K	Joback Method
tf	330.08	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.75	J/mol×K	627.31	Joback Method
cpg	514.47	J/mol×K	661.81	Joback Method
cpg	530.17	J/mol×K	696.31	Joback Method
cpg	544.91	J/mol×K	730.81	Joback Method
cpg	558.73	J/mol×K	765.32	Joback Method

cpg	571.71	J/mol×K	799.82	Joback Method
cpg	583.89	J/mol×K	834.32	Joback Method
dvisc	0.0025373	Pa×s	330.08	Joback Method
dvisc	0.0011605	Pa×s	379.62	Joback Method
dvisc	0.0006358	Pa×s	429.16	Joback Method
dvisc	0.0003946	Pa×s	478.69	Joback Method
dvisc	0.0002678	Pa×s	528.23	Joback Method
dvisc	0.0001942	Pa×s	577.77	Joback Method
dvisc	0.0001482	Pa×s	627.31	Joback Method

Sources

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=C30669477&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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

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