(E)-2-Hexyl-cinnamaldehyde

Other names: 2-Hexyl-(E)-cinnamaldehyde
Inchi: InChI=1S/C15H20O/c1-2-3-4-6-11-15(13-16)12-14-9-7-5-8-10-14/h5,7-10,12-13H,2-4,6,1
InchiKey: GUUHFMWKWLOQMM-NTCAYCPXSA-N
Formula: C15H20O
SMILES: CCCCCCC(C=O)=Cc1ccccc1
Mol. weight [g/mol]: 216.32

Physical Properties

Property code	Value	Unit	Source
gf	159.98	kJ/mol	Joback Method
hf	-94.55	kJ/mol	Joback Method
hfus	29.83	kJ/mol	Joback Method
hvap	58.02	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.239		Crippen Method
mcvol	195.720	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	1754.00		NIST Webbook
rinpol	1749.00		NIST Webbook
tb	621.98	K	Joback Method
tc	827.96	K	Joback Method
tf	308.19	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.60	J/mol×K	621.98	Joback Method
cpg	514.24	J/mol×K	656.31	Joback Method
cpg	529.87	J/mol×K	690.64	Joback Method
cpg	544.54	J/mol×K	724.97	Joback Method
cpg	558.31	J/mol×K	759.30	Joback Method
cpg	571.25	J/mol×K	793.63	Joback Method
cpg	583.40	J/mol×K	827.96	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=R411471&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