Propylcinnamic aldehyde

Inchi: InChI=1S/C12H14O/c1-2-6-12(10-13)9-11-7-4-3-5-8-11/h3-5,7-10H,2,6H2,1H3/b12-9+
InchiKey: FMWHWCCEBSGQQV-FMIVXFBMSA-N
Formula: C12H14O
SMILES: CCCC(C=O)=Cc1ccccc1
Mol. weight [g/mol]: 174.24

Physical Properties

Property code	Value	Unit	Source
gf	134.72	kJ/mol	Joback Method
hf	-32.63	kJ/mol	Joback Method
hfus	22.06	kJ/mol	Joback Method
hvap	51.34	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.069		Crippen Method
mcvol	153.450	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	1531.00		NIST Webbook
ripol	2111.00		NIST Webbook
tb	553.34	K	Joback Method
tc	769.64	K	Joback Method
tf	274.38	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.00	J/mol×K	553.34	Joback Method
cpg	364.94	J/mol×K	589.39	Joback Method
cpg	378.91	J/mol×K	625.44	Joback Method
cpg	391.94	J/mol×K	661.49	Joback Method
cpg	404.11	J/mol×K	697.54	Joback Method
cpg	415.47	J/mol×K	733.59	Joback Method
cpg	426.07	J/mol×K	769.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R410181&Units=SI
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

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