p-Pentyloxycinnamic acid

Inchi: InChI=1S/C14H18O3/c1-2-3-4-11-17-13-8-5-12(6-9-13)7-10-14(15)16/h5-10H,2-4,11H2,1
InchiKey: WXPBGFBUVHLMSK-JXMROGBWSA-N
Formula: C14H18O3
SMILES: CCCCCOc1ccc(C=CC(=O)O)cc1
Mol. weight [g/mol]: 234.29
CAS: 62718-63-2

Physical Properties

Property code	Value	Unit	Source
gf	-120.74	kJ/mol	Joback Method
hf	-387.04	kJ/mol	Joback Method
hfus	32.74	kJ/mol	Joback Method
hvap	75.49	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.353		Crippen Method
mcvol	193.370	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
tb	724.01	K	Joback Method
tc	921.62	K	Joback Method
tf	414.38	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.94	J/mol×K	724.01	Joback Method
cpg	542.69	J/mol×K	756.95	Joback Method
cpg	554.70	J/mol×K	789.88	Joback Method
cpg	565.98	J/mol×K	822.82	Joback Method
cpg	576.57	J/mol×K	855.75	Joback Method
cpg	586.51	J/mol×K	888.69	Joback Method
cpg	595.82	J/mol×K	921.62	Joback Method
dvisc	0.0012903	Pa×s	414.38	Joback Method
dvisc	0.0004832	Pa×s	465.99	Joback Method

dvisc	0.0002201	Pa×s	517.59	Joback Method
dvisc	0.0001156	Pa×s	569.19	Joback Method
dvisc	0.0000676	Pa×s	620.80	Joback Method
dvisc	0.0000429	Pa×s	672.40	Joback Method
dvisc	0.0000291	Pa×s	724.01	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=C62718632&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/38-404-1/p-Pentyloxycinnamic-acid.pdf

Generated by Cheméo on 2024-10-12 07:50:16.436541218 +0000 UTC m=+3300279.073510473.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.