

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,
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/molxK	724.01	Joback Method
cpg	542.69	J/molxK	756.95	Joback Method
cpg	554.70	J/molxK	789.88	Joback Method
cpg	565.98	J/molxK	822.82	Joback Method
cpg	576.57	J/molxK	855.75	Joback Method
cpg	586.51	J/molxK	888.69	Joback Method
cpg	595.82	J/molxK	921.62	Joback Method
dvisc	0.0012903	Paxs	414.38	Joback Method
dvisc	0.0004832	Paxs	465.99	Joback Method

dvisc	0.0002201	Paxs	517.59	Joback Method
dvisc	0.0001156	Paxs	569.19	Joback Method
dvisc	0.0000676	Paxs	620.80	Joback Method
dvisc	0.0000429	Paxs	672.40	Joback Method
dvisc	0.0000291	Paxs	724.01	Joback Method

Sources

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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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