

(Z) Phenylpropyl cinnamate

Inchi:	InChI=1S/C18H18O2/c19-18(14-13-17-10-5-2-6-11-17)20-15-7-12-16-8-3-1-4-9-16/h1-6,
InchiKey:	LYRAHIUDQRJGGZ-YPKPFQOOSA-N
Formula:	C18H18O2
SMILES:	O=C(C=Cc1ccccc1)OCCc1ccccc1
Mol. weight [g/mol]:	266.33

Physical Properties

Property code	Value	Unit	Source
gf	171.80	kJ/mol	Joback Method
hf	-69.37	kJ/mol	Joback Method
hfus	33.45	kJ/mol	Joback Method
hvap	69.33	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.876		Crippen Method
mvol	220.100	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	2195.50		NIST Webbook
rinpol	2195.50		NIST Webbook
tb	745.05	K	Joback Method
tc	978.05	K	Joback Method
tf	412.54	K	Joback Method
vc	0.832	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.39	J/molxK	745.05	Joback Method
cpg	618.52	J/molxK	783.88	Joback Method
cpg	633.41	J/molxK	822.72	Joback Method
cpg	647.13	J/molxK	861.55	Joback Method
cpg	659.78	J/molxK	900.38	Joback Method
cpg	671.42	J/molxK	939.22	Joback Method
cpg	682.16	J/molxK	978.05	Joback Method
dvisc	0.0011452	Paxs	412.54	Joback Method

dvisc	0.0005723	Paxs	467.96	Joback Method
dvisc	0.0003312	Paxs	523.38	Joback Method
dvisc	0.0002129	Paxs	578.80	Joback Method
dvisc	0.0001478	Paxs	634.21	Joback Method
dvisc	0.0001088	Paxs	689.63	Joback Method
dvisc	0.0000838	Paxs	745.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U414291&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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