

«alpha»-Phenylcinnamic acid

Other names:	«alpha»-Stilbenecarboxylic acid Acrylic acid, 2,3-diphenyl- Atropic acid, «beta»-phenyl- Benzeneacetic acid, «alpha»-(phenylmethylene)- Cinnamic acid, «alpha»-phenyl- 2-Phenylcinnamic acid 2-Propenoic acid, 2,3-diphenyl- 2,3-Diphenyl-2-propenoic acid
Inchi:	InChI=1S/C15H12O2/c16-15(17)14(13-9-5-2-6-10-13)11-12-7-3-1-4-8-12/h1-11H,(H,16,17)
InchiKey:	BIDDLNGQCUOJQ-SDNWHVSQSA-N
Formula:	C15H12O2
SMILES:	O=C(O)C(=Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	224.25
CAS:	3368-16-9

Physical Properties

Property code	Value	Unit	Source
gf	106.17	kJ/mol	Joback Method
hf	-37.25	kJ/mol	Joback Method
hfus	27.27	kJ/mol	Joback Method
hvap	77.00	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.312		Crippen Method
mcvol	177.830	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
tb	746.05	K	Joback Method
tc	979.73	K	Joback Method
tf	447.00 ± 3.00	K	NIST Webbook
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.07	J/mol×K	746.05	Joback Method

cpg	481.16	J/mol×K	785.00	Joback Method
cpg	492.28	J/mol×K	823.94	Joback Method
cpg	502.52	J/mol×K	862.89	Joback Method
cpg	511.98	J/mol×K	901.84	Joback Method
cpg	520.75	J/mol×K	940.78	Joback Method
cpg	528.93	J/mol×K	979.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3368169&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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