Benzoic acid, 4-cyano-, phenyl ester

Other names:	Benzoic acid, p-cyano-, phenyl ester
	Phenyl p-cyanobenzoate
	Phenyl 4-cyanobenzoate
	4-Cyanobenzoic acid, phenyl ester
Inchi:	InChI=1S/C14H9NO2/c15-10-11-6-8-12(9-7-11)14(16)17-13-4-2-1-3-5-13/h1-9H
InchiKey:	UTARNPHXZJRNPC-UHFFFAOYSA-N
Formula:	C14H9NO2
SMILES:	N#Cc1ccc(C(=O)Oc2ccccc2)cc1
Mol. weight [g/mol]:	223.23
CAS:	17847-33-5

Physical Properties

Property code	Value	Unit	Source
gf	181.45	kJ/mol	Joback Method
hf	49.38	kJ/mol	Joback Method
hfus	24.00	kJ/mol	Joback Method
hvap	71.61	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	2.777		Crippen Method
mcvol	169.420	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinpol	1883.50		NIST Webbook
tb	756.43	K	Joback Method
tc	1010.63	K	Joback Method
tf	450.05	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.40	J/mol×K	756.43	Joback Method
cpg	444.92	J/mol×K	798.80	Joback Method
cpg	455.34	J/mol×K	841.16	Joback Method
cpg	464.72	J/mol×K	883.53	Joback Method

cpg	473.09	J/mol×K	925.89	Joback Method
cpg	480.53	J/mol×K	968.26	Joback Method
cpg	487.07	J/mol×K	1010.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17847335&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume