Phenylacetic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C15H11NO2/c16-11-13-6-8-14(9-7-13)18-15(17)10-12-4-2-1-3-5-12/h1-9H,10H
InchiKey: YHXBQMXUSPUGEM-UHFFFAOYSA-N
Formula: C15H11NO2
SMILES: N#Cc1ccc(OC(=O)Cc2ccccc2)cc1
Mol. weight [g/mol]: 237.25

Physical Properties

Property code	Value	Unit	Source
gf	189.87	kJ/mol	Joback Method
hf	28.74	kJ/mol	Joback Method
hfus	26.59	kJ/mol	Joback Method
hvap	73.83	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	2.706		Crippen Method
mcvol	183.510	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	1988.00		NIST Webbook
rinpol	1988.00		NIST Webbook
tb	779.31	K	Joback Method
tc	1028.11	K	Joback Method
tf	461.32	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.48	J/mol×K	779.31	Joback Method
cpg	497.46	J/mol×K	820.78	Joback Method
cpg	508.32	J/mol×K	862.24	Joback Method
cpg	518.13	J/mol×K	903.71	Joback Method
cpg	526.92	J/mol×K	945.18	Joback Method
cpg	534.77	J/mol×K	986.65	Joback Method
cpg	541.71	J/mol×K	1028.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307534&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

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