3-Phenylpropionic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C16H13NO2/c17-12-14-6-9-15(10-7-14)19-16(18)11-8-13-4-2-1-3-5-13/h1-7,9-
InchiKey: IAMZBAJGBSDDJE-UHFFFAOYSA-N
Formula: C16H13NO2
SMILES: N#Cc1ccc(OC(=O)CCc2ccccc2)cc1
Mol. weight [g/mol]: 251.28

Physical Properties

Property code	Value	Unit	Source
gf	198.29	kJ/mol	Joback Method
hf	8.10	kJ/mol	Joback Method
hfus	29.18	kJ/mol	Joback Method
hvap	76.06	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.096		Crippen Method
mcvol	197.600	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	2115.00		NIST Webbook
tb	802.19	K	Joback Method
tc	1046.14	K	Joback Method
tf	472.59	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.67	J/mol×K	802.19	Joback Method
cpg	551.02	J/mol×K	842.85	Joback Method
cpg	562.25	J/mol×K	883.51	Joback Method
cpg	572.41	J/mol×K	924.17	Joback Method
cpg	581.55	J/mol×K	964.82	Joback Method
cpg	589.74	J/mol×K	1005.48	Joback Method
cpg	597.03	J/mol×K	1046.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307784&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