3-Cyclopentylpropionic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C15H17NO2/c16-11-13-5-8-14(9-6-13)18-15(17)10-7-12-3-1-2-4-12/h5-6,8-9,1

InchiKey: FJXLIHSGNBYYPJ-UHFFFAOYSA-N

Formula: C15H17NO2

SMILES: N#Cc1ccc(OC(=O)CCC2CCCC2)cc1

Mol. weight [g/mol]: 243.30

Physical Properties

Property code	Value	Unit	Source
gf	114.01	kJ/mol	Joback Method
hf	-147.31	kJ/mol	Joback Method
hfus	26.49	kJ/mol	Joback Method
hvap	71.81	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.434		Crippen Method
mcvol	196.410	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1997.00		NIST Webbook
rinpol	1997.00		NIST Webbook
tb	767.91	K	Joback Method
tc	1003.26	K	Joback Method
tf	445.80	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.74	J/mol×K	767.91	Joback Method
cpg	581.74	J/mol×K	807.14	Joback Method
cpg	595.53	J/mol×K	846.36	Joback Method
cpg	608.17	J/mol×K	885.59	Joback Method
cpg	619.71	J/mol×K	924.81	Joback Method
cpg	630.19	J/mol×K	964.04	Joback Method
cpg	639.67	J/mol×K	1003.26	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307134&Units=SI

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