o-Anisic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C15H11NO3/c1-18-14-5-3-2-4-13(14)15(17)19-12-8-6-11(10-16)7-9-12/h2-9H,
InchiKey: OUGMXEXLTZKKID-UHFFFAOYSA-N
Formula: C15H11NO3
SMILES: COc1ccccc1C(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 253.25

Physical Properties

Property code	Value	Unit	Source
gf	75.24	kJ/mol	Joback Method
hf	-114.95	kJ/mol	Joback Method
hfus	27.39	kJ/mol	Joback Method
hvap	76.90	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	2.786		Crippen Method
mcvol	189.380	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
rinpol	2167.00		NIST Webbook
tb	806.71	K	Joback Method
tc	1052.53	K	Joback Method
tf	496.07	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.38	J/mol×K	806.71	Joback Method
cpg	519.82	J/mol×K	847.68	Joback Method
cpg	530.13	J/mol×K	888.65	Joback Method
cpg	539.32	J/mol×K	929.62	Joback Method
cpg	547.42	J/mol×K	970.59	Joback Method
cpg	554.43	J/mol×K	1011.56	Joback Method
cpg	560.38	J/mol×K	1052.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307793&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

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