o-Toluic acid, 4-cyanophenyl ester

Other names: o-Toluylic acid, 4-cyanophenyl ester
Inchi: InChI=1S/C15H11NO2/c1-11-4-2-3-5-14(11)15(17)18-13-8-6-12(10-16)7-9-13/h2-9H,1H3
InchiKey: FSXGXLHUUDLHFG-UHFFFAOYSA-N
Formula: C15H11NO2
SMILES: Cc1ccccc1C(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 237.25

Physical Properties

Property code	Value	Unit	Source
gf	180.24	kJ/mol	Joback Method
hf	17.27	kJ/mol	Joback Method
hfus	26.20	kJ/mol	Joback Method
hvap	74.49	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.086		Crippen Method
mcvol	183.510	ml/mol	McGowan Method
pc	2487.55	kPa	Joback Method
rinpol	2015.00		NIST Webbook
tb	784.29	K	Joback Method
tc	1033.83	K	Joback Method
tf	473.84	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.85	J/mol×K	784.29	Joback Method
cpg	495.73	J/mol×K	825.88	Joback Method
cpg	506.51	J/mol×K	867.47	Joback Method
cpg	516.24	J/mol×K	909.06	Joback Method
cpg	524.96	J/mol×K	950.65	Joback Method
cpg	532.72	J/mol×K	992.24	Joback Method
cpg	539.55	J/mol×K	1033.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307458&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

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