Benzoic acid, 4-butyl-, 4-cyanophenyl ester

Other names:	p-Cyanophenyl p-butylbenzoate
	4-Cyanophenyl 4-butylbenzoate
	4-Butylbenzoic acid, 4-cyanophenyl ester
Inchi:	InChI=1S/C18H17NO2/c1-2-3-4-14-5-9-16(10-6-14)18(20)21-17-11-7-15(13-19)8-12-17/h
InchiKey:	XQRFASOUJIKXRE-UHFFFAOYSA-N
Formula:	C18H17NO2
SMILES:	CCCCc1ccc(C(=O)Oc2ccc(C#N)cc2)cc1
Mol. weight [g/mol]:	279.33
CAS:	38690-77-6

Physical Properties

Property code	Value	Unit	Source
gf	205.50	kJ/mol	Joback Method
hf	-44.65	kJ/mol	Joback Method
hfus	33.97	kJ/mol	Joback Method
hvap	81.17	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.120		Crippen Method
mcvol	225.780	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
rinpol	2385.00		NIST Webbook
tb	852.93	K	Joback Method
tc	1089.64	K	Joback Method
tf	507.65	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.65	J/mol×K	852.93	Joback Method
cpg	659.47	J/mol×K	892.38	Joback Method
cpg	671.16	J/mol×K	931.83	Joback Method
cpg	681.77	J/mol×K	971.28	Joback Method
cpg	691.34	J/mol×K	1010.73	Joback Method

cpg	699.92	J/mol×K	1050.18	Joback Method
cpg	707.57	J/mol×K	1089.64	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=C38690776&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

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