Isophthalic acid, butyl 4-cyanophenyl ester

Inchi: InChI=1S/C19H17NO4/c1-2-3-11-23-18(21)15-5-4-6-16(12-15)19(22)24-17-9-7-14(13-20
InchiKey: OHJNZUXQDKMZJI-UHFFFAOYSA-N
Formula: C19H17NO4
SMILES: CCCCOC(=O)c1cccc(C(=O)Oc2ccc(C#N)cc2)c1
Mol. weight [g/mol]: 323.34

Physical Properties

Property code	Value	Unit	Source
gf	-20.00	kJ/mol	Joback Method
hf	-310.09	kJ/mol	Joback Method
hfus	39.35	kJ/mol	Joback Method
hvap	92.55	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	3.734		Crippen Method
mcvol	247.310	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	2815.00		NIST Webbook
rinpol	2815.00		NIST Webbook
tb	952.10	K	Joback Method
tc	1190.15	K	Joback Method
tf	591.08	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.74	J/mol×K	952.10	Joback Method
cpg	745.98	J/mol×K	991.77	Joback Method
cpg	754.95	J/mol×K	1031.45	Joback Method
cpg	762.68	J/mol×K	1071.12	Joback Method
cpg	769.20	J/mol×K	1110.80	Joback Method
cpg	774.55	J/mol×K	1150.47	Joback Method
cpg	778.75	J/mol×K	1190.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344489&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