Octanoic acid, 4-cyano-2,6-diiodophenyl ester

Other names:	Benzonitrile, 3,5-diiodo-4-hydroxy-, octanoate
	Benzonitrile, 3,5-diiodo-4-octanoyloxy-
	4-Cyano-2,6-dijodphenol caprysaeureester
	3,5-Diiodo-4-hydroxybenzonitrile octanoate
	3,5-Diiodo-4-octanoyloxybenzonitrile
	3,5-Dijod-4-hydroxy-benzonitril caprysaeureester
	Ioxynil octanoate
	M&B 11,461
	RIP-15830
	Totril
	(4-Cyano-2,6-diiodophenyl) octanoate
Inchi:	InChI=1S/C15H17I2NO2/c1-2-3-4-5-6-7-14(19)20-15-12(16)8-11(10-18)9-13(15)17/h8-9H
InchiKey:	QBEXFUOWUYCXNI-UHFFFAOYSA-N
Formula:	C15H17I2NO2
SMILES:	CCCCCCCC(=O)Oc1c(I)cc(C#N)cc1I
Mol. weight [g/mol]:	497.11
CAS:	3861-47-0

Physical Properties

Property code	Value	Unit	Source
chs	-8019.50	kJ/mol	NIST Webbook
gf	174.44	kJ/mol	Joback Method
hf	-76.99	kJ/mol	Joback Method
hfs	-389.30	kJ/mol	NIST Webbook
hfus	40.58	kJ/mol	Joback Method
hvap	91.63	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	5.033		Crippen Method
mcvol	258.910	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
rinpol	2737.00		NIST Webbook
tb	948.87	K	Joback Method
tc	1200.94	K	Joback Method
tf	576.06	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.60	J/mol×K	948.87	Joback Method
cpg	665.79	J/mol×K	990.88	Joback Method
cpg	675.11	J/mol×K	1032.89	Joback Method
cpg	683.63	J/mol×K	1074.90	Joback Method
cpg	691.40	J/mol×K	1116.92	Joback Method
cpg	698.47	J/mol×K	1158.93	Joback Method
cpg	704.91	J/mol×K	1200.94	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3861470&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

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase 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