2,6-Difluorobenzoic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C14H7F2NO2/c15-11-2-1-3-12(16)13(11)14(18)19-10-6-4-9(8-17)5-7-10/h1-7H
InchiKey: MTEGUFJKGHQFPI-UHFFFAOYSA-N
Formula: C14H7F2NO2
SMILES: N#Cc1ccc(OC(=O)c2c(F)cccc2F)cc1
Mol. weight [g/mol]: 259.21

Physical Properties

Property code	Value	Unit	Source
gf	-227.43	kJ/mol	Joback Method
hf	-365.78	kJ/mol	Joback Method
hfus	29.38	kJ/mol	Joback Method
hvap	71.30	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.056		Crippen Method
mcvol	172.960	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinpol	1879.00		NIST Webbook
tb	764.93	K	Joback Method
tc	999.55	K	Joback Method
tf	476.27	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.59	J/mol×K	764.93	Joback Method
cpg	455.75	J/mol×K	804.03	Joback Method
cpg	465.01	J/mol×K	843.14	Joback Method
cpg	473.38	J/mol×K	882.24	Joback Method
cpg	480.91	J/mol×K	921.34	Joback Method
cpg	487.61	J/mol×K	960.44	Joback Method
cpg	493.51	J/mol×K	999.55	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=U307560&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