2,5-Di(trifluoromethyl)benzoic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C16H7F6NO2/c17-15(18,19)10-3-6-13(16(20,21)22)12(7-10)14(24)25-11-4-1-9

InchiKey: WJHYCQRXQOKJCW-UHFFFAOYSA-N

Formula: C16H7F6NO2

SMILES: N#Cc1ccc(OC(=O)c2cc(C(F)(F)F)ccc2C(F)(F)F)cc1

Mol. weight [g/mol]: 359.22

Physical Properties

Property code	Value	Unit	Source
gf	-984.15	kJ/mol	Joback Method
hf	-1209.00	kJ/mol	Joback Method
hfus	32.06	kJ/mol	Joback Method
hvap	69.89	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	4.815		Crippen Method
mcvol	208.220	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	1855.00		NIST Webbook
rinpol	1855.00		NIST Webbook
tb	801.31	K	Joback Method
tc	1016.66	K	Joback Method
tf	506.01	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.51	J/mol×K	801.31	Joback Method
cpg	594.91	J/mol×K	837.20	Joback Method
cpg	603.46	J/mol×K	873.09	Joback Method
cpg	611.23	J/mol×K	908.99	Joback Method
cpg	618.31	J/mol×K	944.88	Joback Method
cpg	624.75	J/mol×K	980.77	Joback Method
cpg	630.64	J/mol×K	1016.66	Joback Method

Sources

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=U357747&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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