2,5-Di(trifluoromethyl)benzoic acid, 3,5-difluophenyl ester

Inchi: InChI=1S/C15H6F8O2/c16-8-4-9(17)6-10(5-8)25-13(24)11-3-7(14(18,19)20)1-2-12(11)15

InchiKey: MHPYEKPHFUYZRP-UHFFFAOYSA-N

Formula: C15H6F8O2

SMILES: O=C(Oc1cc(F)cc(F)c1)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 370.19

Physical Properties

Property code	Value	Unit	Source
gf	-1525.00	kJ/mol	Joback Method
hf	-1756.93	kJ/mol	Joback Method
hfus	33.73	kJ/mol	Joback Method
hvap	56.21	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.222		Crippen Method
mcvol	196.290	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
rinpol	1471.00		NIST Webbook
tb	679.87	K	Joback Method
tc	871.05	K	Joback Method
tf	443.45	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.74	J/mol×K	679.87	Joback Method
cpg	543.74	J/mol×K	711.73	Joback Method
cpg	553.90	J/mol×K	743.60	Joback Method
cpg	563.28	J/mol×K	775.46	Joback Method
cpg	571.91	J/mol×K	807.32	Joback Method
cpg	579.84	J/mol×K	839.19	Joback Method
cpg	587.13	J/mol×K	871.05	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=U357739&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