2,5-Di(trifluoromethyl)benzoic acid, phenyl ester

Inchi: InChI=1S/C15H8F6O2/c16-14(17,18)9-6-7-12(15(19,20)21)11(8-9)13(22)23-10-4-2-1-3-5

InchiKey: LGJLJNQWHFIDAU-UHFFFAOYSA-N

Formula: C15H8F6O2

SMILES: O=C(Oc1ccccc1)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 334.21

Physical Properties

Property code	Value	Unit	Source
gf	-1116.12	kJ/mol	Joback Method
hf	-1341.77	kJ/mol	Joback Method
hfus	28.35	kJ/mol	Joback Method
hvap	56.52	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.943		Crippen Method
mcvol	192.750	ml/mol	McGowan Method
pc	2043.76	kPa	Joback Method
rinpol	1543.00		NIST Webbook
tb	671.37	K	Joback Method
tc	876.20	K	Joback Method
tf	417.23	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.96	J/mol×K	671.37	Joback Method
cpg	531.33	J/mol×K	705.51	Joback Method
cpg	542.68	J/mol×K	739.65	Joback Method
cpg	553.08	J/mol×K	773.79	Joback Method
cpg	562.61	J/mol×K	807.93	Joback Method
cpg	571.31	J/mol×K	842.06	Joback Method
cpg	579.27	J/mol×K	876.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357741&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

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