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

Inchi: InChI=1S/C15H6Cl2F6O2/c16-10-2-1-3-11(12(10)17)25-13(24)8-6-7(14(18,19)20)4-5-9(8

InchiKey: AEXPPHLWESALGS-UHFFFAOYSA-N

Formula: C15H6Cl2F6O2

SMILES: O=C(Oc1cccc(Cl)c1Cl)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 403.10

Physical Properties

Property code	Value	Unit	Source
gf	-1159.24	kJ/mol	Joback Method
hf	-1396.19	kJ/mol	Joback Method
hfus	35.96	kJ/mol	Joback Method
hvap	66.62	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	6.250		Crippen Method
mcvol	217.230	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	1870.00		NIST Webbook
rinpol	1870.00		NIST Webbook
tb	756.19	K	Joback Method
tc	969.40	K	Joback Method
tf	502.11	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.10	J/mol×K	756.19	Joback Method
cpg	571.81	J/mol×K	791.73	Joback Method
cpg	580.65	J/mol×K	827.26	Joback Method
cpg	588.69	J/mol×K	862.80	Joback Method
cpg	595.99	J/mol×K	898.33	Joback Method
cpg	602.62	J/mol×K	933.87	Joback Method
cpg	608.64	J/mol×K	969.40	Joback Method

Sources

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=U357372&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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