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

Inchi: InChI=1S/C15H7ClF6O2/c16-9-2-4-10(5-3-9)24-13(23)11-7-8(14(17,18)19)1-6-12(11)15(

InchiKey: DNCVWWGBRFGAMZ-UHFFFAOYSA-N

Formula: C15H7ClF6O2

SMILES: O=C(Oc1ccc(Cl)cc1)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 368.66

Physical Properties

Property code	Value	Unit	Source
gf	-1137.68	kJ/mol	Joback Method
hf	-1368.98	kJ/mol	Joback Method
hfus	32.16	kJ/mol	Joback Method
hvap	61.57	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	5.597		Crippen Method
mcvol	204.990	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1726.00		NIST Webbook
rinpol	1726.00		NIST Webbook
tb	713.78	K	Joback Method
tc	922.89	K	Joback Method
tf	459.67	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.72	J/mol×K	713.78	Joback Method
cpg	552.71	J/mol×K	748.63	Joback Method
cpg	562.76	J/mol×K	783.48	Joback Method
cpg	571.93	J/mol×K	818.34	Joback Method
cpg	580.29	J/mol×K	853.19	Joback Method
cpg	587.91	J/mol×K	888.04	Joback Method
cpg	594.86	J/mol×K	922.89	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=U357745&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