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

Inchi: InChI=1S/C16H9ClF6O2/c1-8-6-10(17)3-5-13(8)25-14(24)11-7-9(15(18,19)20)2-4-12(11)16(21,22)23

InchiKey: PRRCJZVSHWUJFH-UHFFFAOYSA-N

Formula: C16H9ClF6O2

SMILES: Cc1cc(Cl)ccc1OC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 382.69

Physical Properties

Property code	Value	Unit	Source
gf	-1138.89	kJ/mol	Joback Method
hf	-1401.09	kJ/mol	Joback Method
hfus	34.36	kJ/mol	Joback Method
hvap	64.46	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	5.905		Crippen Method
mcvol	219.080	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	1797.00		NIST Webbook
tb	741.64	K	Joback Method
tc	949.09	K	Joback Method
tf	483.46	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.97	J/mol×K	741.64	Joback Method
cpg	603.23	J/mol×K	776.21	Joback Method
cpg	613.58	J/mol×K	810.79	Joback Method
cpg	623.07	J/mol×K	845.36	Joback Method
cpg	631.77	J/mol×K	879.94	Joback Method
cpg	639.74	J/mol×K	914.51	Joback Method
cpg	647.05	J/mol×K	949.09	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=U357370&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