2,5-Di(trifluoromethyl)benzoic acid, 2,4-dichloro-6-formylphenyl ester

Inchi: InChI=1S/C16H6Cl2F6O3/c17-9-3-7(6-25)13(12(18)5-9)27-14(26)10-4-8(15(19,20)21)1-2

InchiKey: FJONLBRHBXRTAS-UHFFFAOYSA-N

Formula: C16H6Cl2F6O3

SMILES: O=Cc1cc(Cl)cc(Cl)c1OC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 431.11

Physical Properties

Property code	Value	Unit	Source
gf	-1259.97	kJ/mol	Joback Method
hf	-1513.88	kJ/mol	Joback Method
hfus	40.46	kJ/mol	Joback Method
hvap	76.22	kJ/mol	Joback Method
log10ws	-7.38		Crippen Method
logp	6.063		Crippen Method
mcvol	232.890	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	2054.00		NIST Webbook
tb	832.71	K	Joback Method
tc	1047.45	K	Joback Method
tf	567.90	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.95	J/mol×K	832.71	Joback Method
cpg	628.30	J/mol×K	868.50	Joback Method
cpg	635.87	J/mol×K	904.29	Joback Method
cpg	642.71	J/mol×K	940.08	Joback Method
cpg	648.90	J/mol×K	975.87	Joback Method
cpg	654.49	J/mol×K	1011.66	Joback Method
cpg	659.55	J/mol×K	1047.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357373&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