Dimethylmalonic acid, monochloride, 3,5-difluorophenyl ester

Inchi: InChI=1S/C11H9ClF2O3/c1-11(2,9(12)15)10(16)17-8-4-6(13)3-7(14)5-8/h3-5H,1-2H3
InchiKey: DGSMKEWYOMGZTM-UHFFFAOYSA-N
Formula: C11H9ClF2O3
SMILES: CC(C)(C(=O)Cl)C(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 262.64

Physical Properties

Property code	Value	Unit	Source
gf	-626.66	kJ/mol	Joback Method
hf	-830.87	kJ/mol	Joback Method
hfus	24.84	kJ/mol	Joback Method
hvap	61.04	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	2.662		Crippen Method
mcvol	166.880	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	1384.00		NIST Webbook
tb	650.62	K	Joback Method
tc	865.20	K	Joback Method
tf	420.80	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.57	J/mol×K	650.62	Joback Method
cpg	416.61	J/mol×K	686.38	Joback Method
cpg	426.84	J/mol×K	722.15	Joback Method
cpg	436.31	J/mol×K	757.91	Joback Method
cpg	445.04	J/mol×K	793.68	Joback Method
cpg	453.07	J/mol×K	829.44	Joback Method
cpg	460.43	J/mol×K	865.20	Joback Method

Sources

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=U361817&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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