Pentafluoropropanoic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C11H9F5O2/c1-6-3-7(2)5-8(4-6)18-9(17)10(12,13)11(14,15)16/h3-5H,1-2H3
InchiKey: DTZRJTHRASFXFS-UHFFFAOYSA-N
Formula: C11H9F5O2
SMILES: Cc1cc(C)cc(OC(=O)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 268.18

Physical Properties

Property code	Value	Unit	Source
gf	-1067.40	kJ/mol	Joback Method
hf	-1299.63	kJ/mol	Joback Method
hfus	20.87	kJ/mol	Joback Method
hvap	46.16	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.406		Crippen Method
mcvol	158.380	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
tb	553.90	K	Joback Method
tc	740.92	K	Joback Method
tf	345.14	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.86	J/mol×K	553.90	Joback Method
cpg	406.14	J/mol×K	585.07	Joback Method
cpg	417.62	J/mol×K	616.24	Joback Method
cpg	428.34	J/mol×K	647.41	Joback Method
cpg	438.34	J/mol×K	678.58	Joback Method
cpg	447.65	J/mol×K	709.75	Joback Method
cpg	456.31	J/mol×K	740.92	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=U308002&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume