3-Trifluoromethylcinnamic acid, 2-isopropoxyphenyl ester

Inchi: InChI=1S/C19H17F3O3/c1-13(2)24-16-8-3-4-9-17(16)25-18(23)11-10-14-6-5-7-15(12-14
InchiKey: IKEJVDCAXGPCTA-ZHACJKMWSA-N
Formula: C19H17F3O3
SMILES: CC(C)Oc1ccccc1OC(=O)C=Cc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 350.33

Physical Properties

Property code	Value	Unit	Source
gf	-528.07	kJ/mol	Joback Method
hf	-847.53	kJ/mol	Joback Method
hfus	34.75	kJ/mol	Joback Method
hvap	71.15	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.111		Crippen Method
mcvol	245.370	ml/mol	McGowan Method
pc	1683.79	kPa	Joback Method
rinpol	1994.90		NIST Webbook
tb	794.45	K	Joback Method
tc	1011.74	K	Joback Method
tf	460.27	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.10	J/mol×K	794.45	Joback Method
cpg	722.31	J/mol×K	830.67	Joback Method
cpg	735.41	J/mol×K	866.88	Joback Method
cpg	747.47	J/mol×K	903.10	Joback Method
cpg	758.54	J/mol×K	939.31	Joback Method
cpg	768.70	J/mol×K	975.53	Joback Method
cpg	778.01	J/mol×K	1011.74	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=U292638&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