3-Trifluoromethylcinnamic acid, 2-methylphenyl ester

Inchi: InChI=1S/C17H13F3O2/c1-12-5-2-3-8-15(12)22-16(21)10-9-13-6-4-7-14(11-13)17(18,19
InchiKey: GXXNUUCTTIPXNI-MDZDMXLPSA-N
Formula: C17H13F3O2
SMILES: Cc1ccccc1OC(=O)C=Cc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 306.28

Physical Properties

Property code	Value	Unit	Source
gf	-437.47	kJ/mol	Joback Method
hf	-668.75	kJ/mol	Joback Method
hfus	31.90	kJ/mol	Joback Method
hvap	64.68	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.633		Crippen Method
mcvol	211.320	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
rinpol	1916.20		NIST Webbook
rinpol	1916.20		NIST Webbook
tb	726.71	K	Joback Method
tc	948.48	K	Joback Method
tf	430.50	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.45	J/mol×K	726.71	Joback Method
cpg	586.35	J/mol×K	763.67	Joback Method
cpg	599.15	J/mol×K	800.63	Joback Method
cpg	610.95	J/mol×K	837.60	Joback Method
cpg	621.82	J/mol×K	874.56	Joback Method
cpg	631.84	J/mol×K	911.52	Joback Method
cpg	641.09	J/mol×K	948.48	Joback Method

Sources

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=U292635&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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