trans-3-Trifluoromethylcinnamic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C18H15F3O2/c1-12-8-13(2)10-16(9-12)23-17(22)7-6-14-4-3-5-15(11-14)18(19

InchiKey: PHEVAQCWROUTOW-VOTSOKGWSA-N

Formula: C18H15F3O2

SMILES: Cc1cc(C)cc(OC(=O)C=Cc2cccc(C(F)(F)F)c2)c1

Mol. weight [g/mol]: 320.31

Physical Properties

Property code	Value	Unit	Source
gf	-438.68	kJ/mol	Joback Method
hf	-700.86	kJ/mol	Joback Method
hfus	34.11	kJ/mol	Joback Method
hvap	67.57	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	4.941		Crippen Method
mcvol	225.410	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
rinpol	2121.00		NIST Webbook
tb	754.57	K	Joback Method
tc	973.81	K	Joback Method
tf	454.29	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.83	J/mol×K	754.57	Joback Method
cpg	638.92	J/mol×K	791.11	Joback Method
cpg	651.95	J/mol×K	827.65	Joback Method
cpg	663.99	J/mol×K	864.19	Joback Method
cpg	675.14	J/mol×K	900.73	Joback Method
cpg	685.44	J/mol×K	937.27	Joback Method
cpg	694.99	J/mol×K	973.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307809&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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