3-Trifluoromethylbenzoic acid, 4-biphenyl ester

Inchi: InChI=1S/C20H13F3O2/c21-20(22,23)17-8-4-7-16(13-17)19(24)25-18-11-9-15(10-12-18)

InchiKey: VMEGFSQDDXJCIY-UHFFFAOYSA-N

Formula: C20H13F3O2

SMILES: O=C(Oc1ccc(-c2ccccc2)cc1)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 342.31

Physical Properties

Property code	Value	Unit	Source
gf	-380.02	kJ/mol	Joback Method
hf	-611.36	kJ/mol	Joback Method
hfus	33.51	kJ/mol	Joback Method
hvap	73.68	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	5.592		Crippen Method
mcvol	234.130	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	2464.00		NIST Webbook
rinpol	2464.00		NIST Webbook
tb	817.87	K	Joback Method
tc	1058.22	K	Joback Method
tf	495.81	K	Joback Method
vc	0.898	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.08	J/mol×K	817.87	Joback Method
cpg	681.54	J/mol×K	857.93	Joback Method
cpg	693.72	J/mol×K	897.99	Joback Method
cpg	704.72	J/mol×K	938.04	Joback Method
cpg	714.67	J/mol×K	978.10	Joback Method
cpg	723.65	J/mol×K	1018.16	Joback Method
cpg	731.79	J/mol×K	1058.22	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=U355147&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