3-Fluoro-5-trifluoromethylbenzoic acid, 2-biphenyl ester

Inchi: InChI=1S/C20H12F4O2/c21-16-11-14(10-15(12-16)20(22,23)24)19(25)26-18-9-5-4-8-17(

InchiKey: MPLIYUSDNTVCPP-UHFFFAOYSA-N

Formula: C20H12F4O2

SMILES: O=C(Oc1ccccc1-c1ccccc1)c1cc(F)cc(C(F)(F)F)c1

Mol. weight [g/mol]: 360.30

Physical Properties

Property code	Value	Unit	Source
gf	-584.46	kJ/mol	Joback Method
hf	-818.94	kJ/mol	Joback Method
hfus	36.20	kJ/mol	Joback Method
hvap	73.52	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	5.731		Crippen Method
mcvol	235.900	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
rinpol	2038.00		NIST Webbook
rinpol	2038.00		NIST Webbook
tb	822.12	K	Joback Method
tc	1054.29	K	Joback Method
tf	508.92	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.25	J/mol×K	822.12	Joback Method
cpg	687.00	J/mol×K	860.81	Joback Method
cpg	698.57	J/mol×K	899.51	Joback Method
cpg	709.04	J/mol×K	938.20	Joback Method
cpg	718.51	J/mol×K	976.90	Joback Method
cpg	727.06	J/mol×K	1015.59	Joback Method
cpg	734.79	J/mol×K	1054.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357346&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

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