2,5-Di(trifluoromethyl)benzoic acid, 2-biphenyl ester

Inchi: InChI=1S/C21H12F6O2/c22-20(23,24)14-10-11-17(21(25,26)27)16(12-14)19(28)29-18-9

InchiKey: YBFZELQXHGAHLK-UHFFFAOYSA-N

Formula: C21H12F6O2

SMILES: O=C(Oc1ccccc1-c1ccccc1)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 410.31

Physical Properties

Property code	Value	Unit	Source
gf	-962.82	kJ/mol	Joback Method
hf	-1240.55	kJ/mol	Joback Method
hfus	37.54	kJ/mol	Joback Method
hvap	72.82	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	6.610		Crippen Method
mcvol	253.530	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpol	2046.00		NIST Webbook
tb	840.31	K	Joback Method
tc	1063.58	K	Joback Method
tf	523.79	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.05	J/mol×K	840.31	Joback Method
cpg	758.15	J/mol×K	877.52	Joback Method
cpg	769.17	J/mol×K	914.73	Joback Method
cpg	779.21	J/mol×K	951.95	Joback Method
cpg	788.39	J/mol×K	989.16	Joback Method
cpg	796.82	J/mol×K	1026.37	Joback Method
cpg	804.59	J/mol×K	1063.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357374&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

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