2,4,5-Trifluoro-3-methoxybenzoic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C21H15F3O4/c1-26-20-18(23)16(11-17(22)19(20)24)21(25)28-15-9-7-14(8-10-

InchiKey: NTVUCQHQPSZTLX-UHFFFAOYSA-N

Formula: C21H15F3O4

SMILES: COc1c(F)c(F)cc(C(=O)Oc2ccc(OCc3ccccc3)cc2)c1F

Mol. weight [g/mol]: 388.34

Physical Properties

Property code	Value	Unit	Source
gf	-613.33	kJ/mol	Joback Method
hf	-922.10	kJ/mol	Joback Method
hfus	44.73	kJ/mol	Joback Method
hvap	84.00	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	4.911		Crippen Method
mcvol	259.960	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	2856.00		NIST Webbook
rinpol	2856.00		NIST Webbook
tb	903.76	K	Joback Method
tc	1130.35	K	Joback Method
tf	586.68	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.61	J/mol×K	903.76	Joback Method
cpg	782.29	J/mol×K	941.52	Joback Method
cpg	792.61	J/mol×K	979.29	Joback Method
cpg	801.57	J/mol×K	1017.05	Joback Method
cpg	809.19	J/mol×K	1054.82	Joback Method
cpg	815.48	J/mol×K	1092.58	Joback Method
cpg	820.45	J/mol×K	1130.35	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=U357621&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