2-Fluoro-6-trifluoromethylbenzoic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C21H14F4O3/c22-18-8-4-7-17(21(23,24)25)19(18)20(26)28-16-11-9-15(10-12-

InchiKey: QEBQRWZQVIAWNA-UHFFFAOYSA-N

Formula: C21H14F4O3

SMILES: O=C(Oc1ccc(OCc2ccccc2)cc1)c1c(F)cccc1C(F)(F)F

Mol. weight [g/mol]: 390.33

Physical Properties

Property code	Value	Unit	Source
gf	-681.04	kJ/mol	Joback Method
hf	-971.80	kJ/mol	Joback Method
hfus	39.98	kJ/mol	Joback Method
hvap	78.16	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	5.643		Crippen Method
mcvol	255.860	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	2615.00		NIST Webbook
rinpol	2615.00		NIST Webbook
tb	867.42	K	Joback Method
tc	1094.88	K	Joback Method
tf	542.42	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.82	J/mol×K	867.42	Joback Method
cpg	768.15	J/mol×K	905.33	Joback Method
cpg	779.27	J/mol×K	943.24	Joback Method
cpg	789.25	J/mol×K	981.15	Joback Method
cpg	798.16	J/mol×K	1019.06	Joback Method
cpg	806.08	J/mol×K	1056.97	Joback Method
cpg	813.07	J/mol×K	1094.88	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357702&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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