4-Fluoro-2-trifluoromethylbenzoic acid, phenyl ester

Inchi: InChI=1S/C14H8F4O2/c15-9-6-7-11(12(8-9)14(16,17)18)13(19)20-10-4-2-1-3-5-10/h1-8H

InchiKey: GIGNLSGQERIZQX-UHFFFAOYSA-N

Formula: C14H8F4O2

SMILES: O=C(Oc1ccccc1)c1ccc(F)cc1C(F)(F)F

Mol. weight [g/mol]: 284.21

Physical Properties

Property code	Value	Unit	Source
gf	-737.76	kJ/mol	Joback Method
hf	-920.16	kJ/mol	Joback Method
hfus	27.01	kJ/mol	Joback Method
hvap	57.23	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.064		Crippen Method
mcvol	175.120	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1593.00		NIST Webbook
tb	653.18	K	Joback Method
tc	868.14	K	Joback Method
tf	402.36	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.52	J/mol×K	653.18	Joback Method
cpg	462.17	J/mol×K	689.01	Joback Method
cpg	473.82	J/mol×K	724.83	Joback Method
cpg	484.53	J/mol×K	760.66	Joback Method
cpg	494.35	J/mol×K	796.49	Joback Method
cpg	503.33	J/mol×K	832.31	Joback Method
cpg	511.53	J/mol×K	868.14	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357661&Units=SI

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