2-Fluoro-3-trifluoromethylbenzoic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C14H7ClF4O2/c15-8-4-6-9(7-5-8)21-13(20)10-2-1-3-11(12(10)16)14(17,18)19/

InchiKey: NJRDLFVOYCFHMV-UHFFFAOYSA-N

Formula: C14H7ClF4O2

SMILES: O=C(Oc1ccc(Cl)cc1)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 318.65

Physical Properties

Property code	Value	Unit	Source
gf	-759.32	kJ/mol	Joback Method
hf	-947.37	kJ/mol	Joback Method
hfus	30.82	kJ/mol	Joback Method
hvap	62.27	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.717		Crippen Method
mcvol	187.360	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
rinpol	1865.00		NIST Webbook
rinpol	1865.00		NIST Webbook
tb	695.59	K	Joback Method
tc	914.60	K	Joback Method
tf	444.80	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.13	J/mol×K	695.59	Joback Method
cpg	483.43	J/mol×K	732.09	Joback Method
cpg	493.80	J/mol×K	768.59	Joback Method
cpg	503.28	J/mol×K	805.09	Joback Method
cpg	511.92	J/mol×K	841.59	Joback Method
cpg	519.78	J/mol×K	878.10	Joback Method
cpg	526.90	J/mol×K	914.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357647&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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