2-Trifluoromethylbenzoic acid, 3,5-difluorophenyl ester

Inchi: InChI=1S/C14H7F5O2/c15-8-5-9(16)7-10(6-8)21-13(20)11-3-1-2-4-12(11)14(17,18)19/h1
InchiKey: KZBUKYOPXCWIMY-UHFFFAOYSA-N
Formula: C14H7F5O2
SMILES: O=C(Oc1cc(F)cc(F)c1)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 302.20

Physical Properties

Property code	Value	Unit	Source
gf	-942.20	kJ/mol	Joback Method
hf	-1127.74	kJ/mol	Joback Method
hfus	29.70	kJ/mol	Joback Method
hvap	57.07	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.203		Crippen Method
mcvol	176.890	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	1607.00		NIST Webbook
rinpol	1607.00		NIST Webbook
tb	657.43	K	Joback Method
tc	864.10	K	Joback Method
tf	415.47	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.51	J/mol×K	657.43	Joback Method
cpg	468.38	J/mol×K	691.87	Joback Method
cpg	479.35	J/mol×K	726.32	Joback Method
cpg	489.48	J/mol×K	760.76	Joback Method
cpg	498.79	J/mol×K	795.21	Joback Method
cpg	507.35	J/mol×K	829.65	Joback Method
cpg	515.17	J/mol×K	864.10	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=U299008&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

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