2-Trifluoromethylbenzoic acid, 2-methyl ester

Inchi: InChI=1S/C15H11F3O2/c1-10-6-2-5-9-13(10)20-14(19)11-7-3-4-8-12(11)15(16,17)18/h2-
InchiKey: LBWANXZXSXOKPI-UHFFFAOYSA-N
Formula: C15H11F3O2
SMILES: Cc1ccccc1OC(=O)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 280.24

Physical Properties

Property code	Value	Unit	Source
gf	-534.53	kJ/mol	Joback Method
hf	-744.69	kJ/mol	Joback Method
hfus	26.52	kJ/mol	Joback Method
hvap	60.27	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.233		Crippen Method
mcvol	187.440	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	1767.00		NIST Webbook
tb	676.79	K	Joback Method
tc	897.71	K	Joback Method
tf	413.04	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.84	J/mol×K	676.79	Joback Method
cpg	505.60	J/mol×K	713.61	Joback Method
cpg	518.28	J/mol×K	750.43	Joback Method
cpg	529.94	J/mol×K	787.25	Joback Method
cpg	540.64	J/mol×K	824.07	Joback Method
cpg	550.43	J/mol×K	860.89	Joback Method
cpg	559.37	J/mol×K	897.71	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=U299010&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