

2-Trifluoromethylbenzoic acid, 3-methylphenyl ester

Inchi:	InChI=1S/C15H11F3O2/c1-10-5-4-6-11(9-10)20-14(19)12-7-2-3-8-13(12)15(16,17)18/h2
InchiKey:	RPMLOIJPJHZQOV-UHFFFAOYSA-N
Formula:	C15H11F3O2
SMILES:	<chem>Cc1cccc(OC(=O)c2ccccc2C(F)(F)F)c1</chem>
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	1714.00		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/molxK	676.79	Joback Method
cpg	505.60	J/molxK	713.61	Joback Method
cpg	518.28	J/molxK	750.43	Joback Method
cpg	529.94	J/molxK	787.25	Joback Method
cpg	540.64	J/molxK	824.07	Joback Method
cpg	550.43	J/molxK	860.89	Joback Method
cpg	559.37	J/molxK	897.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307668&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
mccvol:	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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