

3,5-Dimethylphenyl 2,2,2-trifluoroacetate

Other names:	Trifluoroacetic acid, 3,5-dimethylphenyl ester
Inchi:	InChI=1S/C10H9F3O2/c1-6-3-7(2)5-8(4-6)15-9(14)10(11,12)13/h3-5H,1-2H3
InchiKey:	CDSQTRNMTYWKEC-UHFFFAOYSA-N
Formula:	C10H9F3O2
SMILES:	<chem>Cc1cc(C)cc(OC(=O)C(F)(F)F)c1</chem>
Mol. weight [g/mol]:	218.17

Physical Properties

Property code	Value	Unit	Source
gf	-689.04	kJ/mol	Joback Method
hf	-878.02	kJ/mol	Joback Method
hfus	19.53	kJ/mol	Joback Method
hvap	46.86	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.771		Crippen Method
mcvol	140.750	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
rinpol	1059.00		NIST Webbook
rinpol	1059.00		NIST Webbook
tb	535.71	K	Joback Method
tc	732.30	K	Joback Method
tf	330.27	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.31	J/molxK	535.71	Joback Method
cpg	340.22	J/molxK	568.48	Joback Method
cpg	351.43	J/molxK	601.24	Joback Method
cpg	361.97	J/molxK	634.01	Joback Method
cpg	371.86	J/molxK	666.77	Joback Method
cpg	381.13	J/molxK	699.54	Joback Method
cpg	389.79	J/molxK	732.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373263&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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