

2,3,4-trifluorobenzoic acid, 3-chloroprop-2-enyl ester

Inchi:	InChI=1S/C10H6ClF3O2/c11-4-1-5-16-10(15)6-2-3-7(12)9(14)8(6)13/h1-4H,5H2/b4-1+
InchiKey:	GAXBRMYVJHBNHQ-DAFODLJHSA-N
Formula:	C10H6ClF3O2
SMILES:	O=C(OC/C=C/Cl)c1ccc(F)c(F)c1F
Mol. weight [g/mol]:	250.60

Physical Properties

Property code	Value	Unit	Source
hfus	30.96	kJ/mol	Joback Method
logp	3.013		Crippen Method
mcvol	148.690	ml/mol	McGowan Method
rinpol	1485.40		NIST Webbook
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.83	J/mol×K	585.51	Joback Method
cpg	338.49	J/mol×K	618.69	Joback Method
cpg	347.60	J/mol×K	651.87	Joback Method
cpg	356.18	J/mol×K	685.05	Joback Method
cpg	364.24	J/mol×K	718.23	Joback Method
cpg	371.80	J/mol×K	751.41	Joback Method
cpg	378.87	J/mol×K	784.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292561&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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