

Carbonic acid, allyl 3,5-difluorophenyl ester

Inchi:	InChI=1S/C10H8F2O3/c1-2-3-14-10(13)15-9-5-7(11)4-8(12)6-9/h2,4-6H,1,3H2
InchiKey:	SJMUAEDTGGWNEF-UHFFFAOYSA-N
Formula:	C10H8F2O3
SMILES:	C=CCOC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]:	214.17

Physical Properties

Property code	Value	Unit	Source
gf	-514.23	kJ/mol	Joback Method
hf	-679.95	kJ/mol	Joback Method
hfus	23.77	kJ/mol	Joback Method
hvap	50.72	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.666		Crippen Method
mcvol	140.550	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
rinpol	1237.00		NIST Webbook
tb	558.77	K	Joback Method
tc	755.64	K	Joback Method
tf	347.73	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.48	J/mol×K	558.77	Joback Method
cpg	331.35	J/mol×K	591.58	Joback Method
cpg	341.70	J/mol×K	624.39	Joback Method
cpg	351.52	J/mol×K	657.20	Joback Method
cpg	360.81	J/mol×K	690.02	Joback Method
cpg	369.57	J/mol×K	722.83	Joback Method
cpg	377.80	J/mol×K	755.64	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357803&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
hvac:	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

Latest version available from:

<https://www.chemeo.com/cid/22-527-2/Carbonic-acid-allyl-3-5-difluophenyl-ester.pdf>

Generated by Cheméo on 2025-12-05 15:13:27.291111869 +0000 UTC m=+4695804.821152530.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.