

Carbonic acid, propyl 3,5-difluorophenyl ester

Inchi:	InChI=1S/C10H10F2O3/c1-2-3-14-10(13)15-9-5-7(11)4-8(12)6-9/h4-6H,2-3H2,1H3
InchiKey:	OWGIOIYZQQRGHP-UHFFFAOYSA-N
Formula:	C10H10F2O3
SMILES:	CCCOC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]:	216.18

Physical Properties

Property code	Value	Unit	Source
gf	-602.07	kJ/mol	Joback Method
hf	-805.38	kJ/mol	Joback Method
hfus	25.05	kJ/mol	Joback Method
hvap	51.39	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.890		Crippen Method
mcvol	144.850	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
rinpola	1247.00		NIST Webbook
tb	562.09	K	Joback Method
tc	755.21	K	Joback Method
tf	349.49	K	Joback Method
vc	0.566	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.99	J/mol×K	562.09	Joback Method
cpg	351.54	J/mol×K	594.28	Joback Method
cpg	362.57	J/mol×K	626.46	Joback Method
cpg	373.08	J/mol×K	658.65	Joback Method
cpg	383.05	J/mol×K	690.84	Joback Method
cpg	392.48	J/mol×K	723.02	Joback Method
cpg	401.38	J/mol×K	755.21	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=U357815&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
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

Latest version available from:

<https://www.chemeo.com/cid/43-304-6/Carbonic-acid-propyl-3-5-difluophenyl-ester.pdf>

Generated by Cheméo on 2024-04-27 19:04:34.564556596 +0000 UTC m=+16533923.485133925.

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