

Isopropyl-2,4,5-trichloro carbanilate

Inchi:	InChI=1S/C10H10Cl3NO2/c1-5(2)16-10(15)14-9-4-7(12)6(11)3-8(9)13/h3-5H,1-2H3,(H,1
InchiKey:	KBPISZYZLAIVBF-UHFFFAOYSA-N
Formula:	C10H10Cl3NO2
SMILES:	CC(C)OC(=O)Nc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	282.55
CAS:	52819-37-1

Physical Properties

Property code	Value	Unit	Source
gf	-65.92	kJ/mol	Joback Method
hf	-291.44	kJ/mol	Joback Method
hfus	31.48	kJ/mol	Joback Method
hvap	70.47	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.604		Crippen Method
mcvol	182.140	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
tb	708.13	K	Joback Method
tc	937.85	K	Joback Method
tf	466.02	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.61	J/molxK	708.13	Joback Method
cpg	427.06	J/molxK	746.42	Joback Method
cpg	436.74	J/molxK	784.70	Joback Method
cpg	445.66	J/molxK	822.99	Joback Method
cpg	453.83	J/molxK	861.28	Joback Method
cpg	461.27	J/molxK	899.57	Joback Method
cpg	467.98	J/molxK	937.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52819371&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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