

Cyclopropanecarboxylic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi:	InChI=1S/C10H6Cl4O2/c11-5-3-6(12)9(8(14)7(5)13)16-10(15)4-1-2-4/h3-4H,1-2H2
InchiKey:	SCFFYKVQJXROAN-UHFFFAOYSA-N
Formula:	C10H6Cl4O2
SMILES:	O=C(Oc1c(Cl)cc(Cl)c(Cl)c1Cl)C1CC1
Mol. weight [g/mol]:	299.96

Physical Properties

Property code	Value	Unit	Source
gf	-113.68	kJ/mol	Joback Method
hf	-294.04	kJ/mol	Joback Method
hfus	31.85	kJ/mol	Joback Method
hvap	69.39	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.616		Crippen Method
mcvol	173.540	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
rinpol	1954.00		NIST Webbook
tb	707.55	K	Joback Method
tc	953.78	K	Joback Method
tf	488.74	K	Joback Method
vc	0.664	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.69	J/mol×K	707.55	Joback Method
cpg	382.05	J/mol×K	748.59	Joback Method
cpg	390.67	J/mol×K	789.63	Joback Method
cpg	398.59	J/mol×K	830.66	Joback Method
cpg	405.87	J/mol×K	871.70	Joback Method
cpg	412.53	J/mol×K	912.74	Joback Method
cpg	418.64	J/mol×K	953.78	Joback Method
dvisc	0.0012729	Paxs	488.74	Joback Method
dvisc	0.0010114	Paxs	525.21	Joback Method

dvisc	0.0008281	Paxs	561.68	Joback Method
dvisc	0.0006947	Paxs	598.14	Joback Method
dvisc	0.0005947	Paxs	634.61	Joback Method
dvisc	0.0005177	Paxs	671.08	Joback Method
dvisc	0.0004572	Paxs	707.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354665&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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