

Cyclopropanecarboxylic acid, 3,4-dichlorophenyl ester

Inchi:	InChI=1S/C10H8Cl2O2/c11-8-4-3-7(5-9(8)12)14-10(13)6-1-2-6/h3-6H,1-2H2
InchiKey:	IPQDLGFOBIGXHR-UHFFFAOYSA-N
Formula:	C10H8Cl2O2
SMILES:	O=C(Oc1ccc(Cl)c(Cl)c1)C1CC1
Mol. weight [g/mol]:	231.07

Physical Properties

Property code	Value	Unit	Source
gf	-70.56	kJ/mol	Joback Method
hf	-239.62	kJ/mol	Joback Method
hfus	24.24	kJ/mol	Joback Method
hvap	59.29	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.309		Crippen Method
mcvol	149.060	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
rinpol	1634.00		NIST Webbook
tb	622.73	K	Joback Method
tc	861.84	K	Joback Method
tf	403.86	K	Joback Method
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.58	J/molxK	622.73	Joback Method
cpg	383.87	J/molxK	821.99	Joback Method
cpg	375.36	J/molxK	782.14	Joback Method
cpg	366.13	J/molxK	742.29	Joback Method
cpg	356.12	J/molxK	702.43	Joback Method
cpg	345.29	J/molxK	662.58	Joback Method
cpg	391.71	J/molxK	861.84	Joback Method
dvisc	0.0004879	Paxs	622.73	Joback Method
dvisc	0.0005599	Paxs	586.25	Joback Method

dvisc	0.0006544	Paxs	549.77	Joback Method
dvisc	0.0007821	Paxs	513.30	Joback Method
dvisc	0.0009604	Paxs	476.82	Joback Method
dvisc	0.0012201	Paxs	440.34	Joback Method
dvisc	0.0016187	Paxs	403.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307526&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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