

Cyclopropanecarbonyl chloride, 2-phenyl-, trans-

Other names:	trans-2-Phenylcyclopropane-1-carboxylic acid chloride Cyclopropanecarbonyl chloride, 2-phenyl-, (E)- 2-Phenylcyclopropanecarbonyl chloride, trans- trans-2-Phenyl-1-cyclopropanecarbonyl chloride 2-Phenylcyclopropanecarbonyl chloride trans-2-phenylcyclopropanecarbonyl chloride
Inchi:	InChI=1S/C10H9ClO/c11-10(12)9-6-8(9)7-4-2-1-3-5-7/h1-5,8-9H,6H2
InchiKey:	SODZBMGDYKEZJG-UHFFFAOYSA-N
Formula:	C10H9ClO
SMILES:	O=C(Cl)C1CC1c1ccccc1
Mol. weight [g/mol]:	180.63
CAS:	939-87-7

Physical Properties

Property code	Value	Unit	Source
gf	57.92	kJ/mol	Joback Method
hf	-89.06	kJ/mol	Joback Method
hfus	20.70	kJ/mol	Joback Method
hvap	50.86	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.555		Crippen Method
mcvol	130.950	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
rinpol	1415.00		NIST Webbook
rinpol	1415.00		NIST Webbook
tb	548.25	K	Joback Method
tc	785.16	K	Joback Method
tf	322.43	K	Joback Method
vc	0.498	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.98	J/mol×K	548.25	Joback Method

cpg	304.21	J/molxK	587.74	Joback Method
cpg	317.32	J/molxK	627.22	Joback Method
cpg	329.40	J/molxK	666.71	Joback Method
cpg	340.52	J/molxK	706.19	Joback Method
cpg	350.74	J/molxK	745.68	Joback Method
cpg	360.15	J/molxK	785.16	Joback Method
dvisc	0.0021337	Paxs	322.43	Joback Method
dvisc	0.0015735	Paxs	360.07	Joback Method
dvisc	0.0012292	Paxs	397.70	Joback Method
dvisc	0.0010022	Paxs	435.34	Joback Method
dvisc	0.0008441	Paxs	472.98	Joback Method
dvisc	0.0007291	Paxs	510.61	Joback Method
dvisc	0.0006426	Paxs	548.25	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	382.20	K	0.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C939877&Units=SI
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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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