

Diphenylacetyl chloride

Other names:	2,2-Diphenylacetyl chloride Benzeneacetyl chloride, «alpha»-phenyl- Acetyl chloride, diphenyl- Diphenylacetic acid chloride «alpha», «alpha»-Diphenylacetyl chloride Dpac «alpha»-phenylbenzeneacetyl chloride
Inchi:	InChI=1S/C14H11ClO/c15-14(16)13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,13H
InchiKey:	MSYLETHDEIJMAF-UHFFFAOYSA-N
Formula:	C14H11ClO
SMILES:	O=C(Cl)C(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	230.69
CAS:	1871-76-7

Physical Properties

Property code	Value	Unit	Source
gf	148.53	kJ/mol	Joback Method
hf	7.17	kJ/mol	Joback Method
hfus	22.37	kJ/mol	Joback Method
hvap	62.05	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.584		Crippen Method
mcvol	174.410	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
tb	663.94	K	Joback Method
tc	918.88	K	Joback Method
tf	365.23	K	Joback Method
vc	0.652	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.90	J/mol×K	663.94	Joback Method
cpg	431.67	J/mol×K	706.43	Joback Method

cpg	445.10	J/molxK	748.92	Joback Method
cpg	457.29	J/molxK	791.41	Joback Method
cpg	468.34	J/molxK	833.90	Joback Method
cpg	478.35	J/molxK	876.39	Joback Method
cpg	487.40	J/molxK	918.88	Joback Method
dvisc	0.0023700	Paxs	365.23	Joback Method
dvisc	0.0011693	Paxs	415.02	Joback Method
dvisc	0.0006712	Paxs	464.80	Joback Method
dvisc	0.0004290	Paxs	514.59	Joback Method
dvisc	0.0002967	Paxs	564.37	Joback Method
dvisc	0.0002178	Paxs	614.15	Joback Method
dvisc	0.0001675	Paxs	663.94	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	448.70	K	2.30	NIST Webbook
tbrp	451.20	K	2.00	NIST Webbook

Sources

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=C1871767&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	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
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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