

Phenol, 3,5-dichloro-, acetate

Other names:	Acetic acid, 3,5-dichlorophenyl ester
Inchi:	InChI=1S/C8H6Cl2O2/c1-5(11)12-8-3-6(9)2-7(10)4-8/h2-4H,1H3
InchiKey:	DPHLEWZTIXLUGZ-UHFFFAOYSA-N
Formula:	C8H6Cl2O2
SMILES:	CC(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	205.04
CAS:	61925-86-8

Physical Properties

Property code	Value	Unit	Source
gf	-148.15	kJ/mol	Joback Method
hf	-271.14	kJ/mol	Joback Method
hfus	20.92	kJ/mol	Joback Method
hvap	54.93	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.919		Crippen Method
mcvol	131.740	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
rinpol	1334.00		NIST Webbook
rinpol	1334.00		NIST Webbook
rinpol	1367.00		NIST Webbook
ripol	1964.00		NIST Webbook
ripol	1964.00		NIST Webbook
tb	570.23	K	Joback Method
tc	801.88	K	Joback Method
tf	363.38	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.56	J/molxK	570.23	Joback Method
cpg	267.98	J/molxK	608.84	Joback Method
cpg	276.81	J/molxK	647.45	Joback Method

cpg	285.07	J/molxK	686.06	Joback Method
cpg	292.76	J/molxK	724.66	Joback Method
cpg	299.89	J/molxK	763.27	Joback Method
cpg	306.45	J/molxK	801.88	Joback Method
dvisc	0.0013093	Paxs	363.38	Joback Method
dvisc	0.0008718	Paxs	397.86	Joback Method
dvisc	0.0006194	Paxs	432.33	Joback Method
dvisc	0.0004628	Paxs	466.81	Joback Method
dvisc	0.0003600	Paxs	501.28	Joback Method
dvisc	0.0002892	Paxs	535.75	Joback Method
dvisc	0.0002386	Paxs	570.23	Joback Method

Sources

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=C61925868&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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