

2-Chloroethyl phenyl acetate

Inchi:	InChI=1S/C10H11ClO2/c11-6-7-13-10(12)8-9-4-2-1-3-5-9/h1-5H,6-8H2
InchiKey:	IFAWZYKLULDJQC-UHFFFAOYSA-N
Formula:	C10H11ClO2
SMILES:	O=C(Cc1ccccc1)OCCCl
Mol. weight [g/mol]:	198.65
CAS:	943-59-9

Physical Properties

Property code	Value	Unit	Source
gf	-100.12	kJ/mol	Joback Method
hf	-273.74	kJ/mol	Joback Method
hfus	22.68	kJ/mol	Joback Method
hvap	53.67	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.011		Crippen Method
mcvol	147.680	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
tb	568.60	K	Joback Method
tc	785.73	K	Joback Method
tf	330.96	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.61	J/molxK	568.60	Joback Method
cpg	382.82	J/molxK	749.54	Joback Method
cpg	373.06	J/molxK	713.35	Joback Method
cpg	362.58	J/molxK	677.16	Joback Method
cpg	351.36	J/molxK	640.98	Joback Method
cpg	339.38	J/molxK	604.79	Joback Method
cpg	391.88	J/molxK	785.73	Joback Method
dvisc	0.0002148	Paxs	568.60	Joback Method
dvisc	0.0002732	Paxs	528.99	Joback Method

dvisc	0.0003612	Paxs	489.39	Joback Method
dvisc	0.0005016	Paxs	449.78	Joback Method
dvisc	0.0007421	Paxs	410.17	Joback Method
dvisc	0.0011940	Paxs	370.57	Joback Method
dvisc	0.0021527	Paxs	330.96	Joback Method

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=C943599&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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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