

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/mol×K	568.60	Joback Method
cpg	339.38	J/mol×K	604.79	Joback Method
cpg	351.36	J/mol×K	640.98	Joback Method
cpg	362.58	J/mol×K	677.16	Joback Method
cpg	373.06	J/mol×K	713.35	Joback Method
cpg	382.82	J/mol×K	749.54	Joback Method
cpg	391.88	J/mol×K	785.73	Joback Method
dvisc	0.0021527	Pa×s	330.96	Joback Method
dvisc	0.0011940	Pa×s	370.57	Joback Method

dvisc	0.0007421	Pa×s	410.17	Joback Method
dvisc	0.0005016	Pa×s	449.78	Joback Method
dvisc	0.0003612	Pa×s	489.39	Joback Method
dvisc	0.0002732	Pa×s	528.99	Joback Method
dvisc	0.0002148	Pa×s	568.60	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/ci990307l

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

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