p-(2-Chloroethoxy)benzaldehyde

Inchi: InChI=1S/C9H9ClO2/c10-5-6-12-9-3-1-8(7-11)2-4-9/h1-4,7H,5-6H2
InchiKey: HBHHMVNKQWECIS-UHFFFAOYSA-N
Formula: C9H9ClO2
SMILES: O=Cc1ccc(OCCCl)cc1
Mol. weight [g/mol]: 184.62
CAS: 54373-15-8

Physical Properties

Property code	Value	Unit	Source
gf	-88.77	kJ/mol	Joback Method
hf	-237.57	kJ/mol	Joback Method
hfus	20.39	kJ/mol	Joback Method
hvap	52.08	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.117		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	545.49	K	Joback Method
tc	762.26	K	Joback Method
tf	324.28	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.18	J/mol×K	545.49	Joback Method
cpg	293.39	J/mol×K	581.62	Joback Method
cpg	303.95	J/mol×K	617.75	Joback Method
cpg	313.88	J/mol×K	653.88	Joback Method
cpg	323.19	J/mol×K	690.01	Joback Method
cpg	331.89	J/mol×K	726.13	Joback Method
cpg	340.01	J/mol×K	762.26	Joback Method
dvisc	0.0019031	Pa×s	324.28	Joback Method
dvisc	0.0011406	Pa×s	361.15	Joback Method

dvisc	0.0007517	Pa×s	398.02	Joback Method
dvisc	0.0005316	Pa×s	434.88	Joback Method
dvisc	0.0003969	Pa×s	471.75	Joback Method
dvisc	0.0003092	Pa×s	508.62	Joback Method
dvisc	0.0002491	Pa×s	545.49	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	419.00 ± 1.00	K	0.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54373158&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

vc: Critical Volume