1,2-Cyclohexanedicarboxylic acid, di(2-chloroethyl) ester

Inchi: InChI=1S/C12H18Cl2O4/c13-5-7-17-11(15)9-3-1-2-4-10(9)12(16)18-8-6-14/h9-10H,1-8H

InchiKey: IKIDGIJIVUSXNH-UHFFFAOYSA-N

Formula: C12H18Cl2O4

SMILES: O=C(OCCCl)C1CCCCC1C(=O)OCCCl

Mol. weight [g/mol]: 297.18

Physical Properties

Property code	Value	Unit	Source
gf	-424.80	kJ/mol	Joback Method
hf	-778.11	kJ/mol	Joback Method
hfus	33.71	kJ/mol	Joback Method
hvap	69.51	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.357		Crippen Method
mcvol	208.440	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	2040.00		NIST Webbook
rinpol	2040.00		NIST Webbook
tb	716.28	K	Joback Method
tc	927.94	K	Joback Method
tf	432.30	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.19	J/mol×K	716.28	Joback Method
cpg	583.57	J/mol×K	751.56	Joback Method
cpg	597.88	J/mol×K	786.83	Joback Method
cpg	611.13	J/mol×K	822.11	Joback Method
cpg	623.32	J/mol×K	857.39	Joback Method
cpg	634.43	J/mol×K	892.66	Joback Method
cpg	644.49	J/mol×K	927.94	Joback Method
dvisc	0.0014288	Pa×s	432.30	Joback Method

dvisc	0.0008269	Pa×s	479.63	Joback Method
dvisc	0.0005279	Pa×s	526.96	Joback Method
dvisc	0.0003629	Pa×s	574.29	Joback Method
dvisc	0.0002641	Pa×s	621.62	Joback Method
dvisc	0.0002011	Pa×s	668.95	Joback Method
dvisc	0.0001587	Pa×s	716.28	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=U340054&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume