1,2-Cyclohexanedicarboxylic acid, 2,3-dichlorophenyl ethyl ester

Inchi: InChI=1S/C16H18Cl2O4/c1-2-21-15(19)10-6-3-4-7-11(10)16(20)22-13-9-5-8-12(17)14(13
InchiKey: ZYCIJDSTPQTINZ-UHFFFAOYSA-N
Formula: C16H18Cl2O4
SMILES: CCOC(=O)C1CCCCC1C(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 345.22

Physical Properties

Property code	Value	Unit	Source
gf	-297.97	kJ/mol	Joback Method
hf	-647.08	kJ/mol	Joback Method
hfus	37.33	kJ/mol	Joback Method
hvap	82.01	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.268		Crippen Method
mcvol	241.040	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	2410.00		NIST Webbook
rinpol	2410.00		NIST Webbook
tb	844.44	K	Joback Method
tc	1080.07	K	Joback Method
tf	528.84	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.04	J/mol×K	844.44	Joback Method
cpg	752.14	J/mol×K	1040.80	Joback Method
cpg	743.84	J/mol×K	1001.53	Joback Method
cpg	734.09	J/mol×K	962.26	Joback Method
cpg	722.88	J/mol×K	922.98	Joback Method
cpg	710.20	J/mol×K	883.71	Joback Method
cpg	758.99	J/mol×K	1080.07	Joback Method
dvisc	0.0000977	Pa×s	844.44	Joback Method

dvisc	0.0001208	Pa×s	791.84	Joback Method
dvisc	0.0001540	Pa×s	739.24	Joback Method
dvisc	0.0002038	Pa×s	686.64	Joback Method
dvisc	0.0002826	Pa×s	634.04	Joback Method
dvisc	0.0004156	Pa×s	581.44	Joback Method
dvisc	0.0006600	Pa×s	528.84	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339841&Units=SI

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