Cyclohexanecarboxylic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C13H14Cl2O2/c14-11-7-6-10(8-12(11)15)17-13(16)9-4-2-1-3-5-9/h6-9H,1-5H2

InchiKey: JMJTVAZCYQSBSD-UHFFFAOYSA-N

Formula: C13H14Cl2O2

SMILES: O=C(Oc1ccc(Cl)c(Cl)c1)C1CCCCC1

Mol. weight [g/mol]: 273.15

Physical Properties

Property code	Value	Unit	Source
gf	-81.60	kJ/mol	Joback Method
hf	-320.02	kJ/mol	Joback Method
hfus	25.71	kJ/mol	Joback Method
hvap	66.49	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.479		Crippen Method
mcvol	191.330	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	1967.00		NIST Webbook
tb	704.18	K	Joback Method
tc	951.50	K	Joback Method
tf	427.11	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.14	J/mol×K	704.18	Joback Method
cpg	554.91	J/mol×K	910.28	Joback Method
cpg	544.05	J/mol×K	869.06	Joback Method
cpg	531.98	J/mol×K	827.84	Joback Method
cpg	518.66	J/mol×K	786.62	Joback Method
cpg	504.06	J/mol×K	745.40	Joback Method
cpg	564.60	J/mol×K	951.50	Joback Method
dvisc	0.0001511	Pa×s	704.18	Joback Method
dvisc	0.0001900	Pa×s	658.00	Joback Method

dvisc	0.0002474	Pa×s	611.82	Joback Method
dvisc	0.0003362	Pa×s	565.64	Joback Method
dvisc	0.0004827	Pa×s	519.47	Joback Method
dvisc	0.0007436	Pa×s	473.29	Joback Method
dvisc	0.0012577	Pa×s	427.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307707&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume