1,2-Cyclohexanedicarboxylic acid, 2-chlorophenyl ethyl ester

Inchi: InChI=1S/C16H19ClO4/c1-2-20-15(18)11-7-3-4-8-12(11)16(19)21-14-10-6-5-9-13(14)17/

InchiKey: FNDHBEDDCVHTDY-UHFFFAOYSA-N

Formula: C16H19ClO4

SMILES: CCOC(=O)C1CCCCC1C(=O)Oc1ccccc1Cl

Mol. weight [g/mol]: 310.77

Physical Properties

Property code	Value	Unit	Source
gf	-276.41	kJ/mol	Joback Method
hf	-619.87	kJ/mol	Joback Method
hfus	33.52	kJ/mol	Joback Method
hvap	76.97	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.615		Crippen Method
mcvol	228.800	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	2199.00		NIST Webbook
rinpol	2199.00		NIST Webbook
tb	802.03	K	Joback Method
tc	1034.41	K	Joback Method
tf	486.40	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.35	J/mol×K	802.03	Joback Method
cpg	737.22	J/mol×K	995.68	Joback Method
cpg	727.13	J/mol×K	956.95	Joback Method
cpg	715.61	J/mol×K	918.22	Joback Method
cpg	702.65	J/mol×K	879.49	Joback Method
cpg	688.24	J/mol×K	840.76	Joback Method
cpg	745.90	J/mol×K	1034.41	Joback Method
dvisc	0.0001095	Pa×s	802.03	Joback Method

dvisc	0.0001373	Pa×s	749.42	Joback Method
dvisc	0.0001781	Pa×s	696.82	Joback Method
dvisc	0.0002411	Pa×s	644.22	Joback Method
dvisc	0.0003444	Pa×s	591.61	Joback Method
dvisc	0.0005274	Pa×s	539.00	Joback Method
dvisc	0.0008856	Pa×s	486.40	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=U339583&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume