1,2-Cyclohexanedicarboxylic acid, 2-chloroethyl hexyl ester

Inchi: InChI=1S/C16H27ClO4/c1-2-3-4-7-11-20-15(18)13-8-5-6-9-14(13)16(19)21-12-10-17/h13
InchiKey: ZQWQNQKPBZBMTF-UHFFFAOYSA-N
Formula: C16H27ClO4
SMILES: CCCCCCOC(=O)C1CCCCC1C(=O)OCCCl
Mol. weight [g/mol]: 318.84

Physical Properties

Property code	Value	Unit	Source
gf	-379.19	kJ/mol	Joback Method
hf	-844.93	kJ/mol	Joback Method
hfus	39.87	kJ/mol	Joback Method
hvap	74.03	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.698		Crippen Method
mcvol	252.560	ml/mol	McGowan Method
pc	1565.99	kPa	Joback Method
rinpol	2156.00		NIST Webbook
rinpol	2156.00		NIST Webbook
tb	770.37	K	Joback Method
tc	970.45	K	Joback Method
tf	447.46	K	Joback Method
vc	0.961	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.94	J/mol×K	770.37	Joback Method
cpg	780.45	J/mol×K	803.72	Joback Method
cpg	796.78	J/mol×K	837.06	Joback Method
cpg	811.93	J/mol×K	870.41	Joback Method
cpg	825.91	J/mol×K	903.76	Joback Method
cpg	838.74	J/mol×K	937.11	Joback Method
cpg	850.43	J/mol×K	970.45	Joback Method
dvisc	0.0012169	Pa×s	447.46	Joback Method

dvisc	0.0006519	Pa×s	501.28	Joback Method
dvisc	0.0003941	Pa×s	555.10	Joback Method
dvisc	0.0002605	Pa×s	608.91	Joback Method
dvisc	0.0001841	Pa×s	662.73	Joback Method
dvisc	0.0001371	Pa×s	716.55	Joback Method
dvisc	0.0001064	Pa×s	770.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U340045&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

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