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

Inchi: InChI=1S/C17H29ClO4/c1-2-3-4-5-8-12-21-16(19)14-9-6-7-10-15(14)17(20)22-13-11-18/
InchiKey: ZCFISICVYITKBS-UHFFFAOYSA-N
Formula: C17H29ClO4
SMILES: CCCCCCCOC(=O)C1CCCCC1C(=O)OCCCl
Mol. weight [g/mol]: 332.86

Physical Properties

Property code	Value	Unit	Source
gf	-370.77	kJ/mol	Joback Method
hf	-865.57	kJ/mol	Joback Method
hfus	42.46	kJ/mol	Joback Method
hvap	76.25	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.088		Crippen Method
mcvol	266.650	ml/mol	McGowan Method
pc	1453.46	kPa	Joback Method
rinpol	2256.00		NIST Webbook
rinpol	2256.00		NIST Webbook
tb	793.25	K	Joback Method
tc	992.56	K	Joback Method
tf	458.73	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.24	J/mol×K	793.25	Joback Method
cpg	838.88	J/mol×K	826.47	Joback Method
cpg	855.30	J/mol×K	859.69	Joback Method
cpg	870.50	J/mol×K	892.90	Joback Method
cpg	884.51	J/mol×K	926.12	Joback Method
cpg	897.33	J/mol×K	959.34	Joback Method
cpg	908.97	J/mol×K	992.56	Joback Method
dvisc	0.0011082	Pa×s	458.73	Joback Method

dvisc	0.0005862	Pa×s	514.48	Joback Method
dvisc	0.0003512	Pa×s	570.24	Joback Method
dvisc	0.0002305	Pa×s	625.99	Joback Method
dvisc	0.0001621	Pa×s	681.74	Joback Method
dvisc	0.0001202	Pa×s	737.50	Joback Method
dvisc	0.0000930	Pa×s	793.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U340046&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