

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

Inchi:	InChI=1S/C20H35ClO4/c1-2-3-4-5-6-7-8-11-15-24-19(22)17-12-9-10-13-18(17)20(23)25
InchiKey:	PUJAQOQDZOIRHH-UHFFFAOYSA-N
Formula:	C20H35ClO4
SMILES:	CCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCCl
Mol. weight [g/mol]:	374.94

Physical Properties

Property code	Value	Unit	Source
gf	-345.51	kJ/mol	Joback Method
hf	-927.49	kJ/mol	Joback Method
hfus	50.23	kJ/mol	Joback Method
hvap	82.93	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	5.259		Crippen Method
mcvol	308.920	ml/mol	McGowan Method
pc	1180.09	kPa	Joback Method
rinpol	2572.00		NIST Webbook
tb	861.89	K	Joback Method
tc	1062.71	K	Joback Method
tf	492.54	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.88	J/molxK	861.89	Joback Method
cpg	1018.82	J/molxK	895.36	Joback Method
cpg	1035.40	J/molxK	928.83	Joback Method
cpg	1050.63	J/molxK	962.30	Joback Method
cpg	1064.53	J/molxK	995.77	Joback Method
cpg	1077.12	J/molxK	1029.24	Joback Method
cpg	1088.43	J/molxK	1062.71	Joback Method
dvisc	0.0008146	Paxs	492.54	Joback Method
dvisc	0.0004161	Paxs	554.10	Joback Method

dvisc	0.0002431	Paxs	615.66	Joback Method
dvisc	0.0001566	Paxs	677.21	Joback Method
dvisc	0.0001086	Paxs	738.77	Joback Method
dvisc	0.0000796	Paxs	800.33	Joback Method
dvisc	0.0000610	Paxs	861.89	Joback Method

Sources

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=U340049&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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

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