

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

Inchi:	InChI=1S/C19H33ClO4/c1-2-3-4-5-6-7-10-14-23-18(21)16-11-8-9-12-17(16)19(22)24-15
InchiKey:	KLGRZMKDNHJDHJ-UHFFFAOYSA-N
Formula:	C19H33ClO4
SMILES:	CCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCCI
Mol. weight [g/mol]:	360.92

Physical Properties

Property code	Value	Unit	Source
gf	-353.93	kJ/mol	Joback Method
hf	-906.85	kJ/mol	Joback Method
hfus	47.64	kJ/mol	Joback Method
hvap	80.70	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.869		Crippen Method
mcvol	294.830	ml/mol	McGowan Method
pc	1261.95	kPa	Joback Method
rinpol	2466.00		NIST Webbook
tb	839.01	K	Joback Method
tc	1038.64	K	Joback Method
tf	481.27	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.28	J/molxK	839.01	Joback Method
cpg	958.13	J/molxK	872.28	Joback Method
cpg	974.67	J/molxK	905.55	Joback Method
cpg	989.91	J/molxK	938.82	Joback Method
cpg	1003.87	J/molxK	972.09	Joback Method
cpg	1016.56	J/molxK	1005.36	Joback Method
cpg	1028.02	J/molxK	1038.64	Joback Method
dvisc	0.0009064	Paxs	481.27	Joback Method
dvisc	0.0004682	Paxs	540.89	Joback Method

dvisc	0.0002758	Paxs	600.52	Joback Method
dvisc	0.0001787	Paxs	660.14	Joback Method
dvisc	0.0001245	Paxs	719.76	Joback Method
dvisc	0.0000916	Paxs	779.39	Joback Method
dvisc	0.0000704	Paxs	839.01	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=U340048&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

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