

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

Inchi:	InChI=1S/C18H31ClO4/c1-2-3-4-5-6-9-13-22-17(20)15-10-7-8-11-16(15)18(21)23-14-12
InchiKey:	TWWCWZSTVJDFMZ-UHFFFAOYSA-N
Formula:	C18H31ClO4
SMILES:	CCCCCCCCOC(=O)C1CCCCC1C(=O)OCCCI
Mol. weight [g/mol]:	346.89

Physical Properties

Property code	Value	Unit	Source
gf	-362.35	kJ/mol	Joback Method
hf	-886.21	kJ/mol	Joback Method
hfus	45.05	kJ/mol	Joback Method
hvap	78.48	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.478		Crippen Method
mcvol	280.740	ml/mol	McGowan Method
pc	1352.64	kPa	Joback Method
tb	816.13	K	Joback Method
tc	1015.27	K	Joback Method
tf	470.00	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.38	J/molxK	816.13	Joback Method
cpg	956.62	J/molxK	982.08	Joback Method
cpg	943.84	J/molxK	948.89	Joback Method
cpg	929.85	J/molxK	915.70	Joback Method
cpg	914.61	J/molxK	882.51	Joback Method
cpg	898.13	J/molxK	849.32	Joback Method
cpg	968.18	J/molxK	1015.27	Joback Method
dvisc	0.0000810	Paxs	816.13	Joback Method
dvisc	0.0001051	Paxs	758.44	Joback Method
dvisc	0.0001423	Paxs	700.75	Joback Method

dvisc	0.0002033	Paxs	643.07	Joback Method
dvisc	0.0003118	Paxs	585.38	Joback Method
dvisc	0.0005250	Paxs	527.69	Joback Method
dvisc	0.0010045	Paxs	470.00	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=U340047&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i

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
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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