1,2-Cyclohexanedicarboxylic acid, 2,3-dichlorophenyl hexyl ester

Inchi: InChI=1S/C20H26Cl2O4/c1-2-3-4-7-13-25-19(23)14-9-5-6-10-15(14)20(24)26-17-12-8-11

InchiKey: WZEVKCBQMUBBAE-UHFFFAOYSA-N

Formula: C20H26Cl2O4

SMILES: CCCCCCOC(=O)C1CCCCC1C(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 401.32

Physical Properties

Property code	Value	Unit	Source
gf	-264.29	kJ/mol	Joback Method
hf	-729.64	kJ/mol	Joback Method
hfus	47.69	kJ/mol	Joback Method
hvap	90.92	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	5.829		Crippen Method
mcvol	297.400	ml/mol	McGowan Method
pc	1427.22	kPa	Joback Method
rinpol	2792.00		NIST Webbook
rinpol	2792.00		NIST Webbook
tb	935.96	K	Joback Method
tc	1163.56	K	Joback Method
tf	573.92	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	927.19	J/mol×K	935.96	Joback Method
cpg	941.16	J/mol×K	973.89	Joback Method
cpg	953.55	J/mol×K	1011.83	Joback Method
cpg	964.37	J/mol×K	1049.76	Joback Method
cpg	973.66	J/mol×K	1087.69	Joback Method
cpg	981.43	J/mol×K	1125.62	Joback Method
cpg	987.71	J/mol×K	1163.56	Joback Method
dvisc	0.0004465	Pa×s	573.92	Joback Method

dvisc	0.0002680	Pa×s	634.26	Joback Method
dvisc	0.0001757	Pa×s	694.60	Joback Method
dvisc	0.0001233	Pa×s	754.94	Joback Method
dvisc	0.0000912	Pa×s	815.28	Joback Method
dvisc	0.0000703	Pa×s	875.62	Joback Method
dvisc	0.0000560	Pa×s	935.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339845&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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