1,2-Cyclohexanedicarboxylic acid, 2,5-dichlorophenyl isohexyl ester

Inchi: InChI=1S/C20H26Cl2O4/c1-13(2)6-5-11-25-19(23)15-7-3-4-8-16(15)20(24)26-18-12-14(2

InchiKey: NQLXACVERYFQEE-UHFFFAOYSA-N

Formula: C20H26Cl2O4

SMILES: CC(C)CCCOC(=O)C1CCCCC1C(=O)Oc1cc(Cl)ccc1Cl

Mol. weight [g/mol]: 401.32

Physical Properties

Property code	Value	Unit	Source
gf	-266.73	kJ/mol	Joback Method
hf	-734.92	kJ/mol	Joback Method
hfus	44.17	kJ/mol	Joback Method
hvap	90.53	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.685		Crippen Method
mcvol	297.400	ml/mol	McGowan Method
pc	1435.89	kPa	Joback Method
rinpol	2680.00		NIST Webbook
rinpol	2680.00		NIST Webbook
tb	935.52	K	Joback Method
tc	1165.44	K	Joback Method
tf	558.92	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	927.66	J/mol×K	935.52	Joback Method
cpg	981.92	J/mol×K	1127.12	Joback Method
cpg	974.23	J/mol×K	1088.80	Joback Method
cpg	964.99	J/mol×K	1050.48	Joback Method
cpg	954.16	J/mol×K	1012.16	Joback Method
cpg	941.73	J/mol×K	973.84	Joback Method
cpg	988.07	J/mol×K	1165.44	Joback Method
dvisc	0.0000511	Pa×s	935.52	Joback Method

dvisc	0.0000649	Pa×s	872.75	Joback Method
dvisc	0.0000856	Pa×s	809.99	Joback Method
dvisc	0.0001183	Pa×s	747.22	Joback Method
dvisc	0.0001735	Pa×s	684.45	Joback Method
dvisc	0.0002748	Pa×s	621.69	Joback Method
dvisc	0.0004826	Pa×s	558.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339800&Units=SI

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