1,2-Cyclohexanedicarboxylic acid, di(2,5-dichlorophenyl) ester

Inchi: InChI=1S/C20H16Cl4O4/c21-11-5-7-15(23)17(9-11)27-19(25)13-3-1-2-4-14(13)20(26)28

InchiKey: HWKLVIFMUMPWAU-UHFFFAOYSA-N

Formula: C20H16Cl4O4

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

Mol. weight [g/mol]: 462.15

Physical Properties

Property code	Value	Unit	Source
gf	-195.00	kJ/mol	Joback Method
hf	-547.53	kJ/mol	Joback Method
hfus	49.35	kJ/mol	Joback Method
hvap	103.29	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	6.618		Crippen Method
mcvol	298.120	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
rinpol	3239.00		NIST Webbook
rinpol	3239.00		NIST Webbook
tb	1047.46	K	Joback Method
tc	1310.12	K	Joback Method
tf	685.22	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.04	J/mol×K	1047.46	Joback Method
cpg	859.53	J/mol×K	1091.24	Joback Method
cpg	865.16	J/mol×K	1135.01	Joback Method
cpg	868.97	J/mol×K	1178.79	Joback Method
cpg	870.99	J/mol×K	1222.57	Joback Method
cpg	871.27	J/mol×K	1266.34	Joback Method
cpg	869.82	J/mol×K	1310.12	Joback Method
dvisc	0.0002413	Pa×s	685.22	Joback Method

dvisc	0.0001623	Pa×s	745.59	Joback Method
dvisc	0.0001159	Pa×s	805.97	Joback Method
dvisc	0.0000867	Pa×s	866.34	Joback Method
dvisc	0.0000674	Pa×s	926.71	Joback Method
dvisc	0.0000540	Pa×s	987.09	Joback Method
dvisc	0.0000444	Pa×s	1047.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339805&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

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