

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

Inchi:	InChI=1S/C23H32Cl2O4/c1-2-3-4-5-6-7-10-15-28-22(26)18-11-8-9-12-19(18)23(27)29-2
InchiKey:	SDOALRVOJIBLAO-UHFFFAOYSA-N
Formula:	C23H32Cl2O4
SMILES:	CCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	443.40

Physical Properties

Property code	Value	Unit	Source
gf	-239.03	kJ/mol	Joback Method
hf	-791.56	kJ/mol	Joback Method
hfus	55.46	kJ/mol	Joback Method
hvap	97.59	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	6.999		Crippen Method
mvol	339.670	ml/mol	McGowan Method
pc	1160.87	kPa	Joback Method
rinpol	3040.00		NIST Webbook
rinpol	3040.00		NIST Webbook
tb	1004.60	K	Joback Method
tc	1234.43	K	Joback Method
tf	607.73	K	Joback Method
vc	1.294	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1106.38	J/molxK	1004.60	Joback Method
cpg	1157.71	J/molxK	1196.13	Joback Method
cpg	1150.74	J/molxK	1157.82	Joback Method
cpg	1142.17	J/molxK	1119.52	Joback Method
cpg	1131.94	J/molxK	1081.21	Joback Method
cpg	1120.02	J/molxK	1042.91	Joback Method
cpg	1163.10	J/molxK	1234.43	Joback Method
dvisc	0.0000360	Paxs	1004.60	Joback Method

dvisc	0.0000456	Paxs	938.45	Joback Method
dvisc	0.0000599	Paxs	872.31	Joback Method
dvisc	0.0000821	Paxs	806.16	Joback Method
dvisc	0.0001192	Paxs	740.02	Joback Method
dvisc	0.0001863	Paxs	673.88	Joback Method
dvisc	0.0003207	Paxs	607.73	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U339804&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

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