

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

Inchi:	InChI=1S/C19H24Cl2O4/c1-2-3-6-11-24-18(22)14-7-4-5-8-15(14)19(23)25-17-12-13(20)3
InchiKey:	GSZDMKNQACOUOZ-UHFFFAOYSA-N
Formula:	C19H24Cl2O4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	387.30

Physical Properties

Property code	Value	Unit	Source
gf	-272.71	kJ/mol	Joback Method
hf	-709.00	kJ/mol	Joback Method
hfus	45.10	kJ/mol	Joback Method
hvap	88.69	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.439		Crippen Method
mvol	283.310	ml/mol	McGowan Method
pc	1536.66	kPa	Joback Method
rinpol	2631.00		NIST Webbook
rinpol	2631.00		NIST Webbook
tb	913.08	K	Joback Method
tc	1141.60	K	Joback Method
tf	562.65	K	Joback Method
vc	1.069	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	868.44	J/molxK	913.08	Joback Method
cpg	882.50	J/molxK	951.17	Joback Method
cpg	895.01	J/molxK	989.25	Joback Method
cpg	905.99	J/molxK	1027.34	Joback Method
cpg	915.45	J/molxK	1065.42	Joback Method
cpg	923.41	J/molxK	1103.51	Joback Method
cpg	929.91	J/molxK	1141.60	Joback Method
dvisc	0.0004952	Paxs	562.65	Joback Method

dvisc	0.0003006	Paxs	621.05	Joback Method
dvisc	0.0001989	Paxs	679.46	Joback Method
dvisc	0.0001404	Paxs	737.87	Joback Method
dvisc	0.0001044	Paxs	796.27	Joback Method
dvisc	0.0000808	Paxs	854.67	Joback Method
dvisc	0.0000646	Paxs	913.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339799&Units=SI
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

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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