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

Inchi: InChI=1S/C18H22Cl2O4/c1-11(2)10-23-17(21)13-5-3-4-6-14(13)18(22)24-16-9-12(19)7-8

InchiKey: PRZLLEOYJKKUJN-UHFFFAOYSA-N

Formula: C18H22Cl2O4

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

Mol. weight [g/mol]: 373.27

Physical Properties

Property code	Value	Unit	Source
gf	-283.57	kJ/mol	Joback Method
hf	-693.64	kJ/mol	Joback Method
hfus	38.99	kJ/mol	Joback Method
hvap	86.08	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.904		Crippen Method
mcvol	269.220	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	2485.00		NIST Webbook
rinpol	2485.00		NIST Webbook
tb	889.76	K	Joback Method
tc	1122.99	K	Joback Method
tf	536.38	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	810.82	J/mol×K	889.76	Joback Method
cpg	866.57	J/mol×K	1084.12	Joback Method
cpg	858.52	J/mol×K	1045.25	Joback Method
cpg	848.93	J/mol×K	1006.37	Joback Method
cpg	837.80	J/mol×K	967.50	Joback Method
cpg	825.10	J/mol×K	928.63	Joback Method
cpg	873.12	J/mol×K	1122.99	Joback Method
dvisc	0.0000679	Pa×s	889.76	Joback Method

dvisc	0.0000858	Pa×s	830.86	Joback Method
dvisc	0.0001123	Pa×s	771.97	Joback Method
dvisc	0.0001536	Pa×s	713.07	Joback Method
dvisc	0.0002224	Pa×s	654.17	Joback Method
dvisc	0.0003464	Pa×s	595.28	Joback Method
dvisc	0.0005947	Pa×s	536.38	Joback Method

Sources

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=U339797&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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