1,2-Cyclohexanedicarboxylic acid, 2,3-dichlorophenyl heptyl ester

Inchi: InChI=1S/C21H28Cl2O4/c1-2-3-4-5-8-14-26-20(24)15-10-6-7-11-16(15)21(25)27-18-13-9

InchiKey: SKLOCCULYRRWTP-UHFFFAOYSA-N

Formula: C21H28Cl2O4

SMILES: CCCCCCCOC(=O)C1CCCCC1C(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 415.35

Physical Properties

Property code	Value	Unit	Source
gf	-255.87	kJ/mol	Joback Method
hf	-750.28	kJ/mol	Joback Method
hfus	50.28	kJ/mol	Joback Method
hvap	93.14	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.219		Crippen Method
mcvol	311.490	ml/mol	McGowan Method
pc	1329.07	kPa	Joback Method
rinpol	2895.00		NIST Webbook
rinpol	2895.00		NIST Webbook
tb	958.84	K	Joback Method
tc	1186.32	K	Joback Method
tf	585.19	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	986.46	J/mol×K	958.84	Joback Method
cpg	1039.85	J/mol×K	1148.40	Joback Method
cpg	1032.31	J/mol×K	1110.49	Joback Method
cpg	1023.23	J/mol×K	1072.58	Joback Method
cpg	1012.58	J/mol×K	1034.67	Joback Method
cpg	1000.33	J/mol×K	996.75	Joback Method
cpg	1045.88	J/mol×K	1186.32	Joback Method
dvisc	0.0000484	Pa×s	958.84	Joback Method

dvisc	0.0000610	Pa×s	896.56	Joback Method
dvisc	0.0000794	Pa×s	834.29	Joback Method
dvisc	0.0001079	Pa×s	772.01	Joback Method
dvisc	0.0001548	Pa×s	709.74	Joback Method
dvisc	0.0002381	Pa×s	647.47	Joback Method
dvisc	0.0004012	Pa×s	585.19	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=U339846&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