1,2-Cyclohexanedicarboxylic acid, heptyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C21H27Cl3O4/c1-2-3-4-5-8-11-27-20(25)15-9-6-7-10-16(15)21(26)28-19-17(23
InchiKey: PYCLWTBLKRIINA-UHFFFAOYSA-N
Formula: C21H27Cl3O4
SMILES: CCCCCCCOC(=O)C1CCCCC1C(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 449.80

Physical Properties

Property code	Value	Unit	Source
gf	-277.43	kJ/mol	Joback Method
hf	-777.49	kJ/mol	Joback Method
hfus	54.09	kJ/mol	Joback Method
hvap	98.19	kJ/mol	Joback Method
log10ws	-7.56		Crippen Method
logp	6.872		Crippen Method
mcvol	323.730	ml/mol	McGowan Method
pc	1280.08	kPa	Joback Method
rinpol	2979.00		NIST Webbook
rinpol	2979.00		NIST Webbook
tb	1001.25	K	Joback Method
tc	1234.52	K	Joback Method
tf	627.63	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1007.09	J/mol×K	1001.25	Joback Method
cpg	1019.15	J/mol×K	1040.13	Joback Method
cpg	1029.53	J/mol×K	1079.01	Joback Method
cpg	1038.25	J/mol×K	1117.88	Joback Method
cpg	1045.33	J/mol×K	1156.76	Joback Method
cpg	1050.81	J/mol×K	1195.64	Joback Method
cpg	1054.70	J/mol×K	1234.52	Joback Method
dvisc	0.0002984	Pa×s	627.63	Joback Method

dvisc	0.0001858	Pa×s	689.90	Joback Method
dvisc	0.0001251	Pa×s	752.17	Joback Method
dvisc	0.0000895	Pa×s	814.44	Joback Method
dvisc	0.0000672	Pa×s	876.71	Joback Method
dvisc	0.0000524	Pa×s	938.98	Joback Method
dvisc	0.0000421	Pa×s	1001.25	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U339812&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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