Isophthalic acid, heptyl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C21H21Cl3O4/c1-2-3-4-5-6-10-27-20(25)14-8-7-9-15(11-14)21(26)28-19-13-17

InchiKey: RQQCRUMVZZOTLQ-UHFFFAOYSA-N

Formula: C21H21Cl3O4

SMILES: CCCCCCCOC(=O)c1cccc(C(=O)Oc2cc(Cl)c(Cl)cc2Cl)c1

Mol. weight [g/mol]: 443.75

Physical Properties

Property code	Value	Unit	Source
gf	-191.39	kJ/mol	Joback Method
hf	-586.41	kJ/mol	Joback Method
hfus	54.84	kJ/mol	Joback Method
hvap	101.01	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	6.993		Crippen Method
mcvol	310.830	ml/mol	McGowan Method
pc	1422.92	kPa	Joback Method
rinpol	3200.00		NIST Webbook
rinpol	3200.00		NIST Webbook
tb	1018.03	K	Joback Method
tc	1255.93	K	Joback Method
tf	663.43	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.28	J/mol×K	1018.03	Joback Method
cpg	933.96	J/mol×K	1216.28	Joback Method
cpg	929.40	J/mol×K	1176.63	Joback Method
cpg	923.58	J/mol×K	1136.98	Joback Method
cpg	916.48	J/mol×K	1097.33	Joback Method
cpg	908.06	J/mol×K	1057.68	Joback Method
cpg	937.30	J/mol×K	1255.93	Joback Method
dvisc	0.0000325	Pa×s	1018.03	Joback Method

dvisc	0.0000399	Pa×s	958.93	Joback Method
dvisc	0.0000504	Pa×s	899.83	Joback Method
dvisc	0.0000658	Pa×s	840.73	Joback Method
dvisc	0.0000893	Pa×s	781.63	Joback Method
dvisc	0.0001274	Pa×s	722.53	Joback Method
dvisc	0.0001938	Pa×s	663.43	Joback Method

Sources

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=U356614&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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