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

Inchi: InChI=1S/C22H23Cl3O4/c1-2-3-4-5-6-7-11-28-21(26)15-9-8-10-16(12-15)22(27)29-20-14
InchiKey: XLQRIGGTPJQUBM-UHFFFAOYSA-N
Formula: C22H23Cl3O4
SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)Oc2cc(Cl)c(Cl)cc2Cl)c1
Mol. weight [g/mol]: 457.77

Physical Properties

Property code	Value	Unit	Source
gf	-182.97	kJ/mol	Joback Method
hf	-607.05	kJ/mol	Joback Method
hfus	57.43	kJ/mol	Joback Method
hvap	103.23	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	7.383		Crippen Method
mcvol	324.920	ml/mol	McGowan Method
pc	1325.20	kPa	Joback Method
rinpol	3304.00		NIST Webbook
rinpol	3304.00		NIST Webbook
tb	1040.91	K	Joback Method
tc	1280.01	K	Joback Method
tf	674.70	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	956.55	J/mol×K	1040.91	Joback Method
cpg	966.37	J/mol×K	1080.76	Joback Method
cpg	974.79	J/mol×K	1120.61	Joback Method
cpg	981.85	J/mol×K	1160.46	Joback Method
cpg	987.59	J/mol×K	1200.31	Joback Method
cpg	992.05	J/mol×K	1240.16	Joback Method
cpg	995.26	J/mol×K	1280.01	Joback Method
dvisc	0.0001729	Pa×s	674.70	Joback Method

dvisc	0.0001125	Pa×s	735.74	Joback Method
dvisc	0.0000782	Pa×s	796.77	Joback Method
dvisc	0.0000572	Pa×s	857.80	Joback Method
dvisc	0.0000437	Pa×s	918.84	Joback Method
dvisc	0.0000345	Pa×s	979.87	Joback Method
dvisc	0.0000280	Pa×s	1040.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356615&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