Isophthalic acid, 2,5-dichlorophenyl octyl ester

Inchi: InChI=1S/C22H24Cl2O4/c1-2-3-4-5-6-7-13-27-21(25)16-9-8-10-17(14-16)22(26)28-20-15

InchiKey: IARPLLCBKIMWIZ-UHFFFAOYSA-N

Formula: C22H24Cl2O4

SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)Oc2cc(Cl)ccc2Cl)c1

Mol. weight [g/mol]: 423.33

Physical Properties

Property code	Value	Unit	Source
gf	-161.41	kJ/mol	Joback Method
hf	-579.84	kJ/mol	Joback Method
hfus	53.62	kJ/mol	Joback Method
hvap	98.19	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	6.730		Crippen Method
mcvol	312.680	ml/mol	McGowan Method
pc	1376.84	kPa	Joback Method
rinpol	3220.00		NIST Webbook
rinpol	3220.00		NIST Webbook
tb	998.50	K	Joback Method
tc	1231.29	K	Joback Method
tf	632.26	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	939.27	J/mol×K	998.50	Joback Method
cpg	950.62	J/mol×K	1037.30	Joback Method
cpg	960.62	J/mol×K	1076.10	Joback Method
cpg	969.29	J/mol×K	1114.89	Joback Method
cpg	976.70	J/mol×K	1153.69	Joback Method
cpg	982.86	J/mol×K	1192.49	Joback Method
cpg	987.84	J/mol×K	1231.29	Joback Method
dvisc	0.0002287	Pa×s	632.26	Joback Method

dvisc	0.0001430	Pa×s	693.30	Joback Method
dvisc	0.0000964	Pa×s	754.34	Joback Method
dvisc	0.0000690	Pa×s	815.38	Joback Method
dvisc	0.0000517	Pa×s	876.42	Joback Method
dvisc	0.0000402	Pa×s	937.46	Joback Method
dvisc	0.0000323	Pa×s	998.50	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=U344704&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