

Isophthalic acid, 2,4-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)28-20-12
InchiKey:	VLRZGMSLJUPWIM-UHFFFAOYSA-N
Formula:	C22H24Cl2O4
SMILES:	CCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)cc2Cl)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
mvol	312.680	ml/mol	McGowan Method
pc	1376.84	kPa	Joback Method
rinpol	3233.00		NIST Webbook
rinpol	3233.00		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/molxK	998.50	Joback Method
cpg	950.62	J/molxK	1037.30	Joback Method
cpg	960.62	J/molxK	1076.10	Joback Method
cpg	969.29	J/molxK	1114.89	Joback Method
cpg	976.70	J/molxK	1153.69	Joback Method
cpg	982.86	J/molxK	1192.49	Joback Method
cpg	987.84	J/molxK	1231.29	Joback Method
dvisc	0.0002287	Paxs	632.26	Joback Method

dvisc	0.0001430	Paxs	693.30	Joback Method
dvisc	0.0000964	Paxs	754.34	Joback Method
dvisc	0.0000690	Paxs	815.38	Joback Method
dvisc	0.0000517	Paxs	876.42	Joback Method
dvisc	0.0000402	Paxs	937.46	Joback Method
dvisc	0.0000323	Paxs	998.50	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=U344412&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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

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