

Isophthalic acid, 2,5-dichlorophenyl nonyl ester

Inchi:	InChI=1S/C23H26Cl2O4/c1-2-3-4-5-6-7-8-14-28-22(26)17-10-9-11-18(15-17)23(27)29-2
InchiKey:	UMITVXGQFBHTED-UHFFFAOYSA-N
Formula:	C23H26Cl2O4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2cc(Cl)ccc2Cl)c1
Mol. weight [g/mol]:	437.36

Physical Properties

Property code	Value	Unit	Source
gf	-152.99	kJ/mol	Joback Method
hf	-600.48	kJ/mol	Joback Method
hfus	56.21	kJ/mol	Joback Method
hvap	100.41	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	7.120		Crippen Method
mvol	326.770	ml/mol	McGowan Method
pc	1283.75	kPa	Joback Method
rinpol	3315.00		NIST Webbook
rinpol	3315.00		NIST Webbook
tb	1021.38	K	Joback Method
tc	1255.57	K	Joback Method
tf	643.53	K	Joback Method
vc	1.254	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.18	J/molxK	1021.38	Joback Method
cpg	1009.59	J/molxK	1060.41	Joback Method
cpg	1019.59	J/molxK	1099.44	Joback Method
cpg	1028.24	J/molxK	1138.48	Joback Method
cpg	1035.58	J/molxK	1177.51	Joback Method
cpg	1041.66	J/molxK	1216.54	Joback Method
cpg	1046.53	J/molxK	1255.57	Joback Method
dvisc	0.0002042	Paxs	643.53	Joback Method

dvisc	0.0001263	Paxs	706.50	Joback Method
dvisc	0.0000845	Paxs	769.48	Joback Method
dvisc	0.0000601	Paxs	832.45	Joback Method
dvisc	0.0000448	Paxs	895.43	Joback Method
dvisc	0.0000348	Paxs	958.40	Joback Method
dvisc	0.0000278	Paxs	1021.38	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=U344705&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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

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