

Isophthalic acid, 2,4-dichlorophenyl pentyl ester

Inchi:	InChI=1S/C19H18Cl2O4/c1-2-3-4-10-24-18(22)13-6-5-7-14(11-13)19(23)25-17-9-8-15(20)
InchiKey:	GQBBPZPFPVANBP-UHFFFAOYSA-N
Formula:	C19H18Cl2O4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)cc2Cl)c1
Mol. weight [g/mol]:	381.25

Physical Properties

Property code	Value	Unit	Source
gf	-186.67	kJ/mol	Joback Method
hf	-517.92	kJ/mol	Joback Method
hfus	45.85	kJ/mol	Joback Method
hvap	91.51	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	5.560		Crippen Method
mvol	270.410	ml/mol	McGowan Method
pc	1726.03	kPa	Joback Method
rinpol	2908.00		NIST Webbook
rinpol	2908.00		NIST Webbook
tb	929.86	K	Joback Method
tc	1163.73	K	Joback Method
tf	598.45	K	Joback Method
vc	1.030	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.86	J/molxK	929.86	Joback Method
cpg	809.13	J/molxK	1124.75	Joback Method
cpg	802.88	J/molxK	1085.77	Joback Method
cpg	795.46	J/molxK	1046.79	Joback Method
cpg	786.84	J/molxK	1007.82	Joback Method
cpg	776.98	J/molxK	968.84	Joback Method
cpg	814.22	J/molxK	1163.73	Joback Method
dvisc	0.0000500	Paxs	929.86	Joback Method

dvisc	0.0000617	Paxs	874.62	Joback Method
dvisc	0.0000784	Paxs	819.39	Joback Method
dvisc	0.0001029	Paxs	764.15	Joback Method
dvisc	0.0001411	Paxs	708.92	Joback Method
dvisc	0.0002039	Paxs	653.69	Joback Method
dvisc	0.0003155	Paxs	598.45	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=U344408&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

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