

Isophthalic acid, 2,4-dichlorophenyl isoheptyl ester

Inchi:	InChI=1S/C20H20Cl2O4/c1-13(2)5-4-10-25-19(23)14-6-3-7-15(11-14)20(24)26-18-9-8-10
InchiKey:	VMYLWAJWBFLGPD-UHFFFAOYSA-N
Formula:	C20H20Cl2O4
SMILES:	CC(C)CCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)cc2Cl)c1
Mol. weight [g/mol]:	395.28

Physical Properties

Property code	Value	Unit	Source
gf	-180.69	kJ/mol	Joback Method
hf	-543.84	kJ/mol	Joback Method
hfus	44.92	kJ/mol	Joback Method
hvap	93.35	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	5.806		Crippen Method
mvol	284.500	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinpol	2970.00		NIST Webbook
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tb	952.30	K	Joback Method
tc	1187.41	K	Joback Method
tf	594.72	K	Joback Method
vc	1.079	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.54	J/molxK	952.30	Joback Method
cpg	866.94	J/molxK	1148.23	Joback Method
cpg	860.79	J/molxK	1109.04	Joback Method
cpg	853.41	J/molxK	1069.86	Joback Method
cpg	844.76	J/molxK	1030.67	Joback Method
cpg	834.82	J/molxK	991.49	Joback Method
cpg	871.89	J/molxK	1187.41	Joback Method
dvisc	0.0000395	Paxs	952.30	Joback Method

dvisc	0.0000495	Paxs	892.70	Joback Method
dvisc	0.0000641	Paxs	833.11	Joback Method
dvisc	0.0000864	Paxs	773.51	Joback Method
dvisc	0.0001223	Paxs	713.91	Joback Method
dvisc	0.0001846	Paxs	654.32	Joback Method
dvisc	0.0003024	Paxs	594.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344409&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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