

Isophthalic acid, 2-chloro-5-methylphenyl pentyl ester

Inchi:	InChI=1S/C20H21ClO4/c1-3-4-5-11-24-19(22)15-7-6-8-16(13-15)20(23)25-18-12-14(2)9-
InchiKey:	QJFXRWOXINUDMB-UHFFFAOYSA-N
Formula:	C20H21ClO4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)Oc2cc(C)ccc2Cl)c1
Mol. weight [g/mol]:	360.83

Physical Properties

Property code	Value	Unit	Source
gf	-166.32	kJ/mol	Joback Method
hf	-522.82	kJ/mol	Joback Method
hfus	44.24	kJ/mol	Joback Method
hvap	89.35	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	5.215		Crippen Method
mcvol	272.260	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
rinpol	2743.00		NIST Webbook
tb	915.31	K	Joback Method
tc	1144.16	K	Joback Method
tf	579.80	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.07	J/molxK	915.31	Joback Method
cpg	814.66	J/molxK	953.45	Joback Method
cpg	825.96	J/molxK	991.59	Joback Method
cpg	836.00	J/molxK	1029.74	Joback Method
cpg	844.79	J/molxK	1067.88	Joback Method
cpg	852.38	J/molxK	1106.02	Joback Method
cpg	858.78	J/molxK	1144.16	Joback Method
dvisc	0.0003394	Paxs	579.80	Joback Method
dvisc	0.0002149	Paxs	635.72	Joback Method

dvisc	0.0001464	Paxs	691.64	Joback Method
dvisc	0.0001057	Paxs	747.56	Joback Method
dvisc	0.0000798	Paxs	803.47	Joback Method
dvisc	0.0000625	Paxs	859.39	Joback Method
dvisc	0.0000505	Paxs	915.31	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=U356566&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

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