

Isophthalic acid, 3-methylphenyl pentyl ester

Inchi:	InChI=1S/C20H22O4/c1-3-4-5-12-23-19(21)16-9-7-10-17(14-16)20(22)24-18-11-6-8-15(2)
InchiKey:	RKMXPYODIRLGFU-UHFFFAOYSA-N
Formula:	C20H22O4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)Oc2cccc(C)c2)c1
Mol. weight [g/mol]:	326.39

Physical Properties

Property code	Value	Unit	Source
gf	-144.76	kJ/mol	Joback Method
hf	-495.61	kJ/mol	Joback Method
hfus	40.43	kJ/mol	Joback Method
hvap	84.30	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	4.561		Crippen Method
mvol	260.020	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	2681.00		NIST Webbook
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tb	872.90	K	Joback Method
tc	1097.43	K	Joback Method
tf	537.36	K	Joback Method
vc	0.988	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.36	J/molxK	872.90	Joback Method
cpg	838.28	J/molxK	1060.01	Joback Method
cpg	829.14	J/molxK	1022.59	Joback Method
cpg	818.81	J/molxK	985.17	Joback Method
cpg	807.26	J/molxK	947.74	Joback Method
cpg	794.45	J/molxK	910.32	Joback Method
cpg	846.26	J/molxK	1097.43	Joback Method
dvisc	0.0000570	Paxs	872.90	Joback Method

dvisc	0.0000716	Paxs	816.98	Joback Method
dvisc	0.0000928	Paxs	761.05	Joback Method
dvisc	0.0001255	Paxs	705.13	Joback Method
dvisc	0.0001788	Paxs	649.21	Joback Method
dvisc	0.0002722	Paxs	593.28	Joback Method
dvisc	0.0004522	Paxs	537.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344518&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

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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