

Isophthalic acid, 3-methylphenyl octyl ester

Inchi:	InChI=1S/C23H28O4/c1-3-4-5-6-7-8-15-26-22(24)19-12-10-13-20(17-19)23(25)27-21-14
InchiKey:	ZLJSPBIQYUZXFY-UHFFFAOYSA-N
Formula:	C23H28O4
SMILES:	CCCCCCCCOC(=O)c1cccc(C(=O)Oc2cccc(C)c2)c1
Mol. weight [g/mol]:	368.47

Physical Properties

Property code	Value	Unit	Source
gf	-119.50	kJ/mol	Joback Method
hf	-557.53	kJ/mol	Joback Method
hfus	48.20	kJ/mol	Joback Method
hvap	90.98	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	5.732		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1369.71	kPa	Joback Method
rinpol	3004.00		NIST Webbook
rinpol	3004.00		NIST Webbook
tb	941.54	K	Joback Method
tc	1164.15	K	Joback Method
tf	571.17	K	Joback Method
vc	1.155	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.96	J/molxK	941.54	Joback Method
cpg	970.23	J/molxK	978.64	Joback Method
cpg	983.14	J/molxK	1015.74	Joback Method
cpg	994.72	J/molxK	1052.85	Joback Method
cpg	1005.01	J/molxK	1089.95	Joback Method
cpg	1014.06	J/molxK	1127.05	Joback Method
cpg	1021.91	J/molxK	1164.15	Joback Method
dvisc	0.0003350	Paxs	571.17	Joback Method

dvisc	0.0001947	Paxs	632.90	Joback Method
dvisc	0.0001247	Paxs	694.63	Joback Method
dvisc	0.0000858	Paxs	756.36	Joback Method
dvisc	0.0000625	Paxs	818.08	Joback Method
dvisc	0.0000476	Paxs	879.81	Joback Method
dvisc	0.0000376	Paxs	941.54	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=U344521&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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