

Isophthalic acid, 3,4-dimethylphenyl heptyl ester

Inchi:	InChI=1S/C23H28O4/c1-4-5-6-7-8-14-26-22(24)19-10-9-11-20(16-19)23(25)27-21-13-12
InchiKey:	HXLPEQCAIISEBN-UHFFFAOYSA-N
Formula:	C23H28O4
SMILES:	CCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(C)c(C)c2)c1
Mol. weight [g/mol]:	368.47

Physical Properties

Property code	Value	Unit	Source
gf	-129.13	kJ/mol	Joback Method
hf	-569.00	kJ/mol	Joback Method
hfus	47.81	kJ/mol	Joback Method
hvap	91.64	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	5.650		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1354.63	kPa	Joback Method
rinpol	3007.00		NIST Webbook
rinpol	3007.00		NIST Webbook
tb	946.52	K	Joback Method
tc	1169.97	K	Joback Method
tf	583.69	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	954.90	J/molxK	946.52	Joback Method
cpg	969.05	J/molxK	983.76	Joback Method
cpg	981.81	J/molxK	1021.00	Joback Method
cpg	993.22	J/molxK	1058.25	Joback Method
cpg	1003.30	J/molxK	1095.49	Joback Method
cpg	1012.10	J/molxK	1132.73	Joback Method
cpg	1019.64	J/molxK	1169.97	Joback Method
dvisc	0.0002992	Paxs	583.69	Joback Method

dvisc	0.0001810	Paxs	644.16	Joback Method
dvisc	0.0001193	Paxs	704.63	Joback Method
dvisc	0.0000840	Paxs	765.11	Joback Method
dvisc	0.0000623	Paxs	825.58	Joback Method
dvisc	0.0000481	Paxs	886.05	Joback Method
dvisc	0.0000384	Paxs	946.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344445&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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