

Isophthalic acid, 3,4-dimethylphenyl isoheptyl ester

Inchi:	InChI=1S/C22H26O4/c1-15(2)7-6-12-25-21(23)18-8-5-9-19(14-18)22(24)26-20-11-10-16
InchiKey:	SFWJPGLOIJPOLS-UHFFFAOYSA-N
Formula:	C22H26O4
SMILES:	<chem>Cc1ccc(OC(=O)c2cccc(C(=O)OCCCC(C)C)c2)cc1C</chem>
Mol. weight [g/mol]:	354.44

Physical Properties

Property code	Value	Unit	Source
gf	-139.99	kJ/mol	Joback Method
hf	-553.64	kJ/mol	Joback Method
hfus	41.70	kJ/mol	Joback Method
hvap	89.03	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.116		Crippen Method
mvol	288.200	ml/mol	McGowan Method
pc	1464.61	kPa	Joback Method
rinpol	2838.00		NIST Webbook
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tb	923.20	K	Joback Method
tc	1148.69	K	Joback Method
tf	557.42	K	Joback Method
vc	1.093	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.19	J/molxK	923.20	Joback Method
cpg	910.39	J/molxK	960.78	Joback Method
cpg	923.21	J/molxK	998.36	Joback Method
cpg	934.66	J/molxK	1035.95	Joback Method
cpg	944.78	J/molxK	1073.53	Joback Method
cpg	953.59	J/molxK	1111.11	Joback Method
cpg	961.14	J/molxK	1148.69	Joback Method
dvisc	0.0003573	Paxs	557.42	Joback Method

dvisc	0.0002076	Paxs	618.38	Joback Method
dvisc	0.0001330	Paxs	679.35	Joback Method
dvisc	0.0000917	Paxs	740.31	Joback Method
dvisc	0.0000669	Paxs	801.27	Joback Method
dvisc	0.0000510	Paxs	862.24	Joback Method
dvisc	0.0000403	Paxs	923.20	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344443&Units=SI

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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