

Isophthalic acid, 3,4-dimethylcyclohexyl pentyl ester

Inchi:	InChI=1S/C21H30O4/c1-4-5-6-12-24-20(22)17-8-7-9-18(14-17)21(23)25-19-11-10-15(2)
InchiKey:	FIUZJZHTCWQPHA-UHFFFAOYSA-N
Formula:	C21H30O4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)OC2CCC(C)C(C)C2)c1
Mol. weight [g/mol]:	346.46

Physical Properties

Property code	Value	Unit	Source
gf	-230.09	kJ/mol	Joback Method
hf	-727.67	kJ/mol	Joback Method
hfus	43.35	kJ/mol	Joback Method
hvap	83.40	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.015		Crippen Method
mvol	287.010	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
rinpol	2681.00		NIST Webbook
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tb	874.33	K	Joback Method
tc	1091.99	K	Joback Method
tf	508.59	K	Joback Method
vc	1.083	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.46	J/molxK	874.33	Joback Method
cpg	1012.51	J/molxK	1055.71	Joback Method
cpg	1001.27	J/molxK	1019.44	Joback Method
cpg	988.46	J/molxK	983.16	Joback Method
cpg	974.07	J/molxK	946.88	Joback Method
cpg	958.08	J/molxK	910.61	Joback Method
cpg	1022.19	J/molxK	1091.99	Joback Method
dvisc	0.0000836	Paxs	874.33	Joback Method

dvisc	0.0001047	Paxs	813.37	Joback Method
dvisc	0.0001362	Paxs	752.42	Joback Method
dvisc	0.0001854	Paxs	691.46	Joback Method
dvisc	0.0002680	Paxs	630.50	Joback Method
dvisc	0.0004193	Paxs	569.55	Joback Method
dvisc	0.0007300	Paxs	508.59	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=U343804&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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