

Isophthalic acid, 3,4-dimethylcyclohexyl isobutyl ester

Inchi:	InChI=1S/C20H28O4/c1-13(2)12-23-19(21)16-6-5-7-17(11-16)20(22)24-18-9-8-14(3)15(4)
InchiKey:	SQABXCZHPURDHQ-UHFFFAOYSA-N
Formula:	C20H28O4
SMILES:	CC(C)COC(=O)c1cccc(C(=O)OC2CCC(C)C(C)C2)c1
Mol. weight [g/mol]:	332.43

Physical Properties

Property code	Value	Unit	Source
gf	-240.95	kJ/mol	Joback Method
hf	-712.31	kJ/mol	Joback Method
hfus	37.24	kJ/mol	Joback Method
hvap	80.79	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.481		Crippen Method
mcvol	272.920	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinpol	2530.00		NIST Webbook
tb	851.01	K	Joback Method
tc	1072.70	K	Joback Method
tf	482.32	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.13	J/molxK	851.01	Joback Method
cpg	954.63	J/molxK	1035.75	Joback Method
cpg	943.15	J/molxK	998.80	Joback Method
cpg	930.08	J/molxK	961.85	Joback Method
cpg	915.40	J/molxK	924.91	Joback Method
cpg	899.09	J/molxK	887.96	Joback Method
cpg	964.51	J/molxK	1072.70	Joback Method
dvisc	0.0000870	Paxs	851.01	Joback Method
dvisc	0.0001101	Paxs	789.56	Joback Method

dvisc	0.0001451	Paxs	728.11	Joback Method
dvisc	0.0002011	Paxs	666.66	Joback Method
dvisc	0.0002978	Paxs	605.22	Joback Method
dvisc	0.0004820	Paxs	543.77	Joback Method
dvisc	0.0008820	Paxs	482.32	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=U343802&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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