

Phthalic acid, di(3-methoxybenzyl) ester

Inchi: InChI=1S/C24H22O6/c1-27-19-9-5-7-17(13-19)15-29-23(25)21-11-3-4-12-22(21)24(26)3
InchiKey: DFMPZCOFANJDFT-UHFFFAOYSA-N
Formula: C24H22O6
SMILES: COc1cccc(COC(=O)c2ccccc2C(=O)OCc2cccc(OC)c2)c1
Mol. weight [g/mol]: 406.43

Physical Properties

Property code	Value	Unit	Source
gf	-218.30	kJ/mol	Joback Method
hf	-617.55	kJ/mol	Joback Method
hfus	46.82	kJ/mol	Joback Method
hvap	100.96	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	4.418		Crippen Method
mvol	304.360	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
rinpol	3267.00		NIST Webbook
rinpol	3267.00		NIST Webbook
tb	1040.92	K	Joback Method
tc	1286.89	K	Joback Method
tf	665.84	K	Joback Method
vc	1.139	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.79	J/molxK	1040.92	Joback Method
cpg	982.11	J/molxK	1245.89	Joback Method
cpg	980.59	J/molxK	1204.90	Joback Method
cpg	977.22	J/molxK	1163.90	Joback Method
cpg	971.97	J/molxK	1122.91	Joback Method
cpg	964.83	J/molxK	1081.91	Joback Method
cpg	981.79	J/molxK	1286.89	Joback Method
dvisc	0.0000191	Paxs	1040.92	Joback Method

dvisc	0.0000237	Paxs	978.41	Joback Method
dvisc	0.0000302	Paxs	915.89	Joback Method
dvisc	0.0000399	Paxs	853.38	Joback Method
dvisc	0.0000552	Paxs	790.87	Joback Method
dvisc	0.0000807	Paxs	728.35	Joback Method
dvisc	0.0001267	Paxs	665.84	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=U377990&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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