

Phthalic acid, isobutyl 3-methoxybenzyl ester

Inchi:	InChI=1S/C20H22O5/c1-14(2)12-24-19(21)17-9-4-5-10-18(17)20(22)25-13-15-7-6-8-16(
InchiKey:	XFILQVWGXXWVPSL-UHFFFAOYSA-N
Formula:	C20H22O5
SMILES:	COc1cccc(COC(=O)c2ccccc2C(=O)OCC(C)C)c1
Mol. weight [g/mol]:	342.39

Physical Properties

Property code	Value	Unit	Source
gf	-252.20	kJ/mol	Joback Method
hf	-633.11	kJ/mol	Joback Method
hfus	38.10	kJ/mol	Joback Method
hvap	86.32	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	3.865		Crippen Method
mcvol	265.890	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinsol	2555.00		NIST Webbook
tb	894.88	K	Joback Method
tc	1121.27	K	Joback Method
tf	544.59	K	Joback Method
vc	1.000	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.05	J/molxK	894.88	Joback Method
cpg	861.40	J/molxK	1083.54	Joback Method
cpg	853.52	J/molxK	1045.81	Joback Method
cpg	844.26	J/molxK	1008.08	Joback Method
cpg	833.60	J/molxK	970.34	Joback Method
cpg	821.54	J/molxK	932.61	Joback Method
cpg	867.92	J/molxK	1121.27	Joback Method
dvisc	0.0000392	Paxs	894.88	Joback Method
dvisc	0.0000497	Paxs	836.50	Joback Method

dvisc	0.0000654	Paxs	778.12	Joback Method
dvisc	0.0000900	Paxs	719.74	Joback Method
dvisc	0.0001308	Paxs	661.35	Joback Method
dvisc	0.0002046	Paxs	602.97	Joback Method
dvisc	0.0003522	Paxs	544.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377976&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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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