Phthalic acid, isobutyl 2-methoxybenzyl ester

Inchi: InChI=1S/C20H22O5/c1-14(2)12-24-19(21)16-9-5-6-10-17(16)20(22)25-13-15-8-4-7-11-1
InchiKey: RUXPYADFFDPPIE-UHFFFAOYSA-N
Formula: C20H22O5
SMILES: COc1ccccc1COC(=O)c1ccccc1C(=O)OCC(C)C
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
rinpol	2912.00		NIST Webbook
rinpol	2912.00		NIST Webbook
tb	894.88	K	Joback Method
tc	1121.27	K	Joback Method
tf	544.59	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.05	J/mol×K	894.88	Joback Method
cpg	821.54	J/mol×K	932.61	Joback Method
cpg	833.60	J/mol×K	970.34	Joback Method
cpg	844.26	J/mol×K	1008.08	Joback Method
cpg	853.52	J/mol×K	1045.81	Joback Method
cpg	861.40	J/mol×K	1083.54	Joback Method
cpg	867.92	J/mol×K	1121.27	Joback Method
dvisc	0.0003522	Pa×s	544.59	Joback Method

dvisc	0.0002046	Pa×s	602.97	Joback Method
dvisc	0.0001308	Pa×s	661.35	Joback Method
dvisc	0.0000900	Pa×s	719.74	Joback Method
dvisc	0.0000654	Pa×s	778.12	Joback Method
dvisc	0.0000497	Pa×s	836.50	Joback Method
dvisc	0.0000392	Pa×s	894.88	Joback Method

Sources

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=U382492&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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