Phthalic acid, 5-bromo-2-methoxybenzyl isobutyl ester

Inchi: InChI=1S/C20H21BrO5/c1-13(2)11-25-19(22)16-6-4-5-7-17(16)20(23)26-12-14-10-15(21

InchiKey: VAFNTFBFKXHXOZ-UHFFFAOYSA-N

Formula: C20H21BrO5

SMILES: COc1ccc(Br)cc1COC(=O)c1ccccc1C(=O)OCC(C)C

Mol. weight [g/mol]: 421.28

Physical Properties

Property code	Value	Unit	Source
gf	-247.51	kJ/mol	Joback Method
hf	-618.25	kJ/mol	Joback Method
hfus	42.99	kJ/mol	Joback Method
hvap	93.42	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	4.627		Crippen Method
mcvol	283.390	ml/mol	McGowan Method
pc	1781.84	kPa	Joback Method
rinpol	2742.00		NIST Webbook
rinpol	2742.00		NIST Webbook
tb	966.02	K	Joback Method
tc	1202.98	K	Joback Method
tf	616.91	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.43	J/mol×K	966.02	Joback Method
cpg	879.91	J/mol×K	1163.49	Joback Method
cpg	874.44	J/mol×K	1123.99	Joback Method
cpg	867.58	J/mol×K	1084.50	Joback Method
cpg	859.30	J/mol×K	1045.01	Joback Method
cpg	849.59	J/mol×K	1005.51	Joback Method
cpg	884.01	J/mol×K	1202.98	Joback Method
dvisc	0.0000313	Pa×s	966.02	Joback Method

dvisc	0.0000389	Pa×s	907.84	Joback Method
dvisc	0.0000498	Pa×s	849.65	Joback Method
dvisc	0.0000662	Pa×s	791.47	Joback Method
dvisc	0.0000921	Pa×s	733.28	Joback Method
dvisc	0.0001355	Pa×s	675.10	Joback Method
dvisc	0.0002145	Pa×s	616.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382865&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