Phthalic acid, butyl 3-methoxybenzyl ester

Inchi: InChI=1S/C20H22O5/c1-3-4-12-24-19(21)17-10-5-6-11-18(17)20(22)25-14-15-8-7-9-16(1
InchiKey: VYQBECNLWYYKAQ-UHFFFAOYSA-N
Formula: C20H22O5
SMILES: CCCCOC(=O)c1ccccc1C(=O)OCc1cccc(OC)c1
Mol. weight [g/mol]: 342.39

Physical Properties

Property code	Value	Unit	Source
gf	-249.76	kJ/mol	Joback Method
hf	-627.83	kJ/mol	Joback Method
hfus	41.62	kJ/mol	Joback Method
hvap	86.71	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.009		Crippen Method
mcvol	265.890	ml/mol	McGowan Method
pc	1692.12	kPa	Joback Method
rinpol	2604.00		NIST Webbook
rinpol	2604.00		NIST Webbook
tb	895.32	K	Joback Method
tc	1119.10	K	Joback Method
tf	559.59	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.52	J/mol×K	895.32	Joback Method
cpg	820.89	J/mol×K	932.62	Joback Method
cpg	832.88	J/mol×K	969.91	Joback Method
cpg	843.50	J/mol×K	1007.21	Joback Method
cpg	852.78	J/mol×K	1044.51	Joback Method
cpg	860.72	J/mol×K	1081.80	Joback Method
cpg	867.35	J/mol×K	1119.10	Joback Method
dvisc	0.0003238	Pa×s	559.59	Joback Method

dvisc	0.0001984	Pa×s	615.55	Joback Method
dvisc	0.0001319	Pa×s	671.50	Joback Method
dvisc	0.0000933	Pa×s	727.45	Joback Method
dvisc	0.0000694	Pa×s	783.41	Joback Method
dvisc	0.0000537	Pa×s	839.37	Joback Method
dvisc	0.0000429	Pa×s	895.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377977&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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