Terephthalic acid, butyl 3-methoxyphenyl ester

Inchi: InChI=1S/C19H20O5/c1-3-4-12-23-18(20)14-8-10-15(11-9-14)19(21)24-17-7-5-6-16(13-1

InchiKey: HXXUYJTYUWDNHU-UHFFFAOYSA-N

Formula: C19H20O5

SMILES: CCCCOC(=O)c1ccc(C(=O)Oc2cccc(OC)c2)cc1

Mol. weight [g/mol]: 328.36

Physical Properties

Property code	Value	Unit	Source
gf	-258.18	kJ/mol	Joback Method
hf	-607.19	kJ/mol	Joback Method
hfus	39.03	kJ/mol	Joback Method
hvap	84.49	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	3.871		Crippen Method
mcvol	251.800	ml/mol	McGowan Method
pc	1834.11	kPa	Joback Method
rinpol	2878.00		NIST Webbook
rinpol	2878.00		NIST Webbook
tb	872.44	K	Joback Method
tc	1097.71	K	Joback Method
tf	548.32	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.17	J/mol×K	872.44	Joback Method
cpg	763.48	J/mol×K	909.98	Joback Method
cpg	775.46	J/mol×K	947.53	Joback Method
cpg	786.10	J/mol×K	985.07	Joback Method
cpg	795.42	J/mol×K	1022.62	Joback Method
cpg	803.43	J/mol×K	1060.16	Joback Method
cpg	810.15	J/mol×K	1097.71	Joback Method
dvisc	0.0003565	Pa×s	548.32	Joback Method

dvisc	0.0002211	Pa×s	602.34	Joback Method
dvisc	0.0001483	Pa×s	656.36	Joback Method
dvisc	0.0001057	Pa×s	710.38	Joback Method
dvisc	0.0000790	Pa×s	764.40	Joback Method
dvisc	0.0000614	Pa×s	818.42	Joback Method
dvisc	0.0000492	Pa×s	872.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415820&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