Isophthalic acid, butyl phenylethyl ester

Inchi: InChI=1S/C20H22O4/c1-2-3-13-23-19(21)17-10-7-11-18(15-17)20(22)24-14-12-16-8-5-4
InchiKey: STDHAVBCKYCQIB-UHFFFAOYSA-N
Formula: C20H22O4
SMILES: CCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)c1
Mol. weight [g/mol]: 326.39

Physical Properties

Property code	Value	Unit	Source
gf	-135.13	kJ/mol	Joback Method
hf	-484.14	kJ/mol	Joback Method
hfus	40.82	kJ/mol	Joback Method
hvap	83.64	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.043		Crippen Method
mcvol	260.020	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	2674.00		NIST Webbook
rinpol	2674.00		NIST Webbook
tb	867.92	K	Joback Method
tc	1091.70	K	Joback Method
tf	524.84	K	Joback Method
vc	0.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.49	J/mol×K	867.92	Joback Method
cpg	840.06	J/mol×K	1054.40	Joback Method
cpg	830.75	J/mol×K	1017.10	Joback Method
cpg	820.28	J/mol×K	979.81	Joback Method
cpg	808.60	J/mol×K	942.51	Joback Method
cpg	795.69	J/mol×K	905.22	Joback Method
cpg	848.25	J/mol×K	1091.70	Joback Method
dvisc	0.0000561	Pa×s	867.92	Joback Method

dvisc	0.0000713	Pa×s	810.74	Joback Method
dvisc	0.0000939	Pa×s	753.56	Joback Method
dvisc	0.0001295	Pa×s	696.38	Joback Method
dvisc	0.0001891	Pa×s	639.20	Joback Method
dvisc	0.0002974	Pa×s	582.02	Joback Method
dvisc	0.0005161	Pa×s	524.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344334&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