Isophthalic acid, butyl 3,4-dimethylphenyl ester

Inchi: InChI=1S/C20H22O4/c1-4-5-11-23-19(21)16-7-6-8-17(13-16)20(22)24-18-10-9-14(2)15(3

InchiKey: BRYHDMJXCUDFTJ-UHFFFAOYSA-N

Formula: C20H22O4

SMILES: CCCCOC(=O)c1cccc(C(=O)Oc2ccc(C)c(C)c2)c1

Mol. weight [g/mol]: 326.39

Physical Properties

Property code	Value	Unit	Source
gf	-154.39	kJ/mol	Joback Method
hf	-507.08	kJ/mol	Joback Method
hfus	40.04	kJ/mol	Joback Method
hvap	84.96	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	4.480		Crippen Method
mcvol	260.020	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinpol	2686.00		NIST Webbook
rinpol	2686.00		NIST Webbook
tb	877.88	K	Joback Method
tc	1103.17	K	Joback Method
tf	549.88	K	Joback Method
vc	0.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.21	J/mol×K	877.88	Joback Method
cpg	793.20	J/mol×K	915.43	Joback Method
cpg	805.90	J/mol×K	952.98	Joback Method
cpg	817.33	J/mol×K	990.52	Joback Method
cpg	827.51	J/mol×K	1028.07	Joback Method
cpg	836.47	J/mol×K	1065.62	Joback Method
cpg	844.23	J/mol×K	1103.17	Joback Method
dvisc	0.0004003	Pa×s	549.88	Joback Method

dvisc	0.0002508	Pa×s	604.55	Joback Method
dvisc	0.0001698	Pa×s	659.21	Joback Method
dvisc	0.0001221	Pa×s	713.88	Joback Method
dvisc	0.0000919	Pa×s	768.55	Joback Method
dvisc	0.0000719	Pa×s	823.21	Joback Method
dvisc	0.0000580	Pa×s	877.88	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=U344441&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