Isophthalic acid, 2,6-dimethoxyphenyl isobutyl ester

Inchi: InChI=1S/C20H22O6/c1-13(2)12-25-19(21)14-7-5-8-15(11-14)20(22)26-18-16(23-3)9-6-1

InchiKey: REHYAMUUOSHTRP-UHFFFAOYSA-N

Formula: C20H22O6

SMILES: COc1cccc(OC)c1OC(=O)c1cccc(C(=O)OCC(C)C)c1

Mol. weight [g/mol]: 358.39

Physical Properties

Property code	Value	Unit	Source
gf	-366.83	kJ/mol	Joback Method
hf	-776.80	kJ/mol	Joback Method
hfus	38.90	kJ/mol	Joback Method
hvap	89.40	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	3.736		Crippen Method
mcvol	271.760	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	2791.00		NIST Webbook
rinpol	2791.00		NIST Webbook
tb	922.28	K	Joback Method
tc	1148.95	K	Joback Method
tf	579.34	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.56	J/mol×K	922.28	Joback Method
cpg	846.05	J/mol×K	960.06	Joback Method
cpg	856.97	J/mol×K	997.84	Joback Method
cpg	866.33	J/mol×K	1035.61	Joback Method
cpg	874.10	J/mol×K	1073.39	Joback Method
cpg	880.27	J/mol×K	1111.17	Joback Method
cpg	884.84	J/mol×K	1148.95	Joback Method
dvisc	0.0002222	Pa×s	579.34	Joback Method

dvisc	0.0001369	Pa×s	636.50	Joback Method
dvisc	0.0000913	Pa×s	693.65	Joback Method
dvisc	0.0000648	Pa×s	750.81	Joback Method
dvisc	0.0000483	Pa×s	807.97	Joback Method
dvisc	0.0000374	Pa×s	865.12	Joback Method
dvisc	0.0000299	Pa×s	922.28	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=U344532&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