Isophthalic acid, isobutyl 1-phenylpropyl ester

Inchi: InChI=1S/C21H24O4/c1-4-19(16-9-6-5-7-10-16)25-21(23)18-12-8-11-17(13-18)20(22)24
InchiKey: LJJOLXHWGOEOGT-UHFFFAOYSA-N
Formula: C21H24O4
SMILES: CCC(OC(=O)c1cccc(C(=O)OCC(C)C)c1)c1ccccc1
Mol. weight [g/mol]: 340.41

Physical Properties

Property code	Value	Unit	Source
gf	-131.59	kJ/mol	Joback Method
hf	-515.34	kJ/mol	Joback Method
hfus	36.37	kJ/mol	Joback Method
hvap	85.09	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.807		Crippen Method
mcvol	274.110	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	2592.00		NIST Webbook
rinpol	2592.00		NIST Webbook
tb	889.92	K	Joback Method
tc	1117.61	K	Joback Method
tf	506.11	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.36	J/mol×K	889.92	Joback Method
cpg	854.90	J/mol×K	927.87	Joback Method
cpg	868.06	J/mol×K	965.82	Joback Method
cpg	879.88	J/mol×K	1003.76	Joback Method
cpg	890.39	J/mol×K	1041.71	Joback Method
cpg	899.65	J/mol×K	1079.66	Joback Method
cpg	907.70	J/mol×K	1117.61	Joback Method
dvisc	0.0005809	Pa×s	506.11	Joback Method

dvisc	0.0002912	Pa×s	570.08	Joback Method
dvisc	0.0001678	Pa×s	634.05	Joback Method
dvisc	0.0001069	Pa×s	698.02	Joback Method
dvisc	0.0000735	Pa×s	761.98	Joback Method
dvisc	0.0000536	Pa×s	825.95	Joback Method
dvisc	0.0000408	Pa×s	889.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344549&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

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