Isophthalic acid, isobutyl 2-isopropylphenyl ester

Inchi: InChI=1S/C21H24O4/c1-14(2)13-24-20(22)16-8-7-9-17(12-16)21(23)25-19-11-6-5-10-18

InchiKey: YOOBMPVRGKBBTK-UHFFFAOYSA-N

Formula: C21H24O4

SMILES: CC(C)COC(=O)c1cccc(C(=O)Oc2ccccc2C(C)C)c1

Mol. weight [g/mol]: 340.41

Physical Properties

Property code	Value	Unit	Source
gf	-141.22	kJ/mol	Joback Method
hf	-526.81	kJ/mol	Joback Method
hfus	35.98	kJ/mol	Joback Method
hvap	85.75	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.842		Crippen Method
mcvol	274.110	ml/mol	McGowan Method
pc	1607.71	kPa	Joback Method
rinpol	2559.00		NIST Webbook
tb	894.90	K	Joback Method
tc	1123.34	K	Joback Method
tf	518.63	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.26	J/mol×K	894.90	Joback Method
cpg	897.79	J/mol×K	1085.27	Joback Method
cpg	888.74	J/mol×K	1047.19	Joback Method
cpg	878.39	J/mol×K	1009.12	Joback Method
cpg	866.72	J/mol×K	971.05	Joback Method
cpg	853.69	J/mol×K	932.97	Joback Method
cpg	905.60	J/mol×K	1123.34	Joback Method
dvisc	0.0000415	Pa×s	894.90	Joback Method
dvisc	0.0000538	Pa×s	832.19	Joback Method

dvisc	0.0000726	Pa×s	769.48	Joback Method
dvisc	0.0001034	Pa×s	706.76	Joback Method
dvisc	0.0001577	Pa×s	644.05	Joback Method
dvisc	0.0002634	Pa×s	581.34	Joback Method
dvisc	0.0004983	Pa×s	518.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344632&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