Isophthalic acid, isobutyl 1-naphthyl ester

Inchi: InChI=1S/C22H20O4/c1-15(2)14-25-21(23)17-9-5-10-18(13-17)22(24)26-20-12-6-8-16-7
InchiKey: PGDHSPBIHGLBAG-UHFFFAOYSA-N
Formula: C22H20O4
SMILES: CC(C)COC(=O)c1cccc(C(=O)Oc2cccc3ccccc23)c1
Mol. weight [g/mol]: 348.39

Physical Properties

Property code	Value	Unit	Source
gf	-23.71	kJ/mol	Joback Method
hf	-351.10	kJ/mol	Joback Method
hfus	39.11	kJ/mol	Joback Method
hvap	90.01	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	4.872		Crippen Method
mcvol	268.740	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	3026.00		NIST Webbook
rinpol	3026.00		NIST Webbook
tb	937.20	K	Joback Method
tc	1178.88	K	Joback Method
tf	577.60	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.45	J/mol×K	937.20	Joback Method
cpg	869.30	J/mol×K	1138.60	Joback Method
cpg	860.88	J/mol×K	1098.32	Joback Method
cpg	851.47	J/mol×K	1058.04	Joback Method
cpg	840.98	J/mol×K	1017.76	Joback Method
cpg	829.33	J/mol×K	977.48	Joback Method
cpg	876.79	J/mol×K	1178.88	Joback Method
dvisc	0.0000811	Pa×s	937.20	Joback Method

dvisc	0.0000996	Pa×s	877.27	Joback Method
dvisc	0.0001261	Pa×s	817.33	Joback Method
dvisc	0.0001657	Pa×s	757.40	Joback Method
dvisc	0.0002283	Pa×s	697.47	Joback Method
dvisc	0.0003340	Pa×s	637.53	Joback Method
dvisc	0.0005287	Pa×s	577.60	Joback Method

Sources

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=U344687&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:
https://www.chemeo.com/cid/72-482-7/Isophthalic-acid-isobutyl-1-naphthyl-ester.pdf
Generated by Cheméo on 2024-04-29 17:33:04.553728694 +0000 UTC m=+16701233.474306005.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.