

Isophthalic acid, butyl 2-isopropoxyphenyl ester

Inchi:	InChI=1S/C21H24O5/c1-4-5-13-24-20(22)16-9-8-10-17(14-16)21(23)26-19-12-7-6-11-18
InchiKey:	RNMVKEBHNRFPV-UHFFFAOYSA-N
Formula:	C21H24O5
SMILES:	CCCCOC(=O)c1cccc(C(=O)Oc2ccccc2OC(C)C)c1
Mol. weight [g/mol]:	356.41

Physical Properties

Property code	Value	Unit	Source
gf	-243.78	kJ/mol	Joback Method
hf	-653.75	kJ/mol	Joback Method
hfus	40.69	kJ/mol	Joback Method
hvap	88.55	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	4.650		Crippen Method
mvol	279.980	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	2690.00		NIST Webbook
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tb	917.76	K	Joback Method
tc	1143.05	K	Joback Method
tf	555.86	K	Joback Method
vc	1.056	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.06	J/molxK	917.76	Joback Method
cpg	919.07	J/molxK	1105.50	Joback Method
cpg	911.31	J/molxK	1067.95	Joback Method
cpg	902.14	J/molxK	1030.40	Joback Method
cpg	891.56	J/molxK	992.86	Joback Method
cpg	879.54	J/molxK	955.31	Joback Method
cpg	925.45	J/molxK	1143.05	Joback Method
dvisc	0.0000340	Paxs	917.76	Joback Method

dvisc	0.0000433	Paxs	857.44	Joback Method
dvisc	0.0000572	Paxs	797.13	Joback Method
dvisc	0.0000790	Paxs	736.81	Joback Method
dvisc	0.0001157	Paxs	676.49	Joback Method
dvisc	0.0001825	Paxs	616.18	Joback Method
dvisc	0.0003177	Paxs	555.86	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=U344428&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

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