

Isophthalic acid, butyl 4-isopropylphenyl ester

Inchi:	InChI=1S/C21H24O4/c1-4-5-13-24-20(22)17-7-6-8-18(14-17)21(23)25-19-11-9-16(10-12
InchiKey:	ULAAYMDQBiyOTA-UHFFFAOYSA-N
Formula:	C21H24O4
SMILES:	CCCCOC(=O)c1cccc(C(=O)Oc2ccc(C(C)C)cc2)c1
Mol. weight [g/mol]:	340.41

Physical Properties

Property code	Value	Unit	Source
gf	-138.78	kJ/mol	Joback Method
hf	-521.53	kJ/mol	Joback Method
hfus	39.50	kJ/mol	Joback Method
hvap	86.14	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	4.986		Crippen Method
mvol	274.110	ml/mol	McGowan Method
pc	1597.44	kPa	Joback Method
rinpol	2772.00		NIST Webbook
rinpol	2772.00		NIST Webbook
tb	895.34	K	Joback Method
tc	1121.05	K	Joback Method
tf	533.63	K	Joback Method
vc	1.038	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.74	J/molxK	895.34	Joback Method
cpg	853.04	J/molxK	932.96	Joback Method
cpg	865.98	J/molxK	970.58	Joback Method
cpg	877.61	J/molxK	1008.19	Joback Method
cpg	887.95	J/molxK	1045.81	Joback Method
cpg	897.05	J/molxK	1083.43	Joback Method
cpg	904.93	J/molxK	1121.05	Joback Method
dvisc	0.0004495	Paxs	533.63	Joback Method

dvisc	0.0002528	Paxs	593.91	Joback Method
dvisc	0.0001581	Paxs	654.20	Joback Method
dvisc	0.0001070	Paxs	714.49	Joback Method
dvisc	0.0000769	Paxs	774.77	Joback Method
dvisc	0.0000580	Paxs	835.06	Joback Method
dvisc	0.0000455	Paxs	895.34	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=U344454&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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