Isophthalic acid, butyl phenyl ester

Inchi: InChI=1S/C18H18O4/c1-2-3-12-21-17(19)14-8-7-9-15(13-14)18(20)22-16-10-5-4-6-11-16
InchiKey: QHXOZNQXFANSFA-UHFFFAOYSA-N
Formula: C18H18O4
SMILES: CCCCOC(=O)c1cccc(C(=O)Oc2ccccc2)c1
Mol. weight [g/mol]: 298.33

Physical Properties

Property code	Value	Unit	Source
gf	-151.97	kJ/mol	Joback Method
hf	-442.86	kJ/mol	Joback Method
hfus	35.64	kJ/mol	Joback Method
hvap	79.19	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	3.863		Crippen Method
mcvol	231.840	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	2473.00		NIST Webbook
rinpol	2473.00		NIST Webbook
tb	822.16	K	Joback Method
tc	1050.77	K	Joback Method
tf	502.30	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.19	J/mol×K	822.16	Joback Method
cpg	682.15	J/mol×K	860.26	Joback Method
cpg	694.86	J/mol×K	898.36	Joback Method
cpg	706.35	J/mol×K	936.47	Joback Method
cpg	716.67	J/mol×K	974.57	Joback Method
cpg	725.84	J/mol×K	1012.67	Joback Method
cpg	733.89	J/mol×K	1050.77	Joback Method
dvisc	0.0006210	Pa×s	502.30	Joback Method

dvisc	0.0003667	Pa×s	555.61	Joback Method
dvisc	0.0002375	Pa×s	608.92	Joback Method
dvisc	0.0001649	Pa×s	662.23	Joback Method
dvisc	0.0001210	Pa×s	715.54	Joback Method
dvisc	0.0000926	Pa×s	768.85	Joback Method
dvisc	0.0000734	Pa×s	822.16	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=U344357&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

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