

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:	QH XOZNQXFANSFA-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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0003667	Paxs	555.61	Joback Method
dvisc	0.0002375	Paxs	608.92	Joback Method
dvisc	0.0001649	Paxs	662.23	Joback Method
dvisc	0.0001210	Paxs	715.54	Joback Method
dvisc	0.0000926	Paxs	768.85	Joback Method
dvisc	0.0000734	Paxs	822.16	Joback Method

Sources

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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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