Isophthalic acid, isobutyl pent-4-enyl ester

Inchi: InChI=1S/C17H22O4/c1-4-5-6-10-20-16(18)14-8-7-9-15(11-14)17(19)21-12-13(2)3/h4,7-
InchiKey: GKKUBJOPDYROQD-UHFFFAOYSA-N
Formula: C17H22O4
SMILES: C=CCCCOC(=O)c1cccc(C(=O)OCC(C)C)c1
Mol. weight [g/mol]: 290.35

Physical Properties

Property code	Value	Unit	Source
gf	-187.40	kJ/mol	Joback Method
hf	-538.60	kJ/mol	Joback Method
hfus	34.21	kJ/mol	Joback Method
hvap	73.63	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.622		Crippen Method
mcvol	237.210	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	2103.00		NIST Webbook
tb	768.84	K	Joback Method
tc	974.59	K	Joback Method
tf	447.85	K	Joback Method
vc	0.902	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.29	J/mol×K	768.84	Joback Method
cpg	694.40	J/mol×K	803.13	Joback Method
cpg	708.49	J/mol×K	837.42	Joback Method
cpg	721.56	J/mol×K	871.72	Joback Method
cpg	733.65	J/mol×K	906.01	Joback Method
cpg	744.77	J/mol×K	940.30	Joback Method
cpg	754.94	J/mol×K	974.59	Joback Method
dvisc	0.0009085	Pa×s	447.85	Joback Method
dvisc	0.0004887	Pa×s	501.35	Joback Method

dvisc	0.0002962	Pa×s	554.85	Joback Method
dvisc	0.0001961	Pa×s	608.35	Joback Method
dvisc	0.0001388	Pa×s	661.84	Joback Method
dvisc	0.0001034	Pa×s	715.34	Joback Method
dvisc	0.0000803	Pa×s	768.84	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=U356713&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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