Isophthalic acid, isobutyl trans-hex-3-enyl ester

Inchi: InChI=1S/C18H24O4/c1-4-5-6-7-11-21-17(19)15-9-8-10-16(12-15)18(20)22-13-14(2)3/h5

InchiKey: ONPSLEDZUBPUGM-AATRIKPKSA-N

Formula: C18H24O4

SMILES: CCC=CCCOC(=O)c1cccc(C(=O)OCC(C)C)c1

Mol. weight [g/mol]: 304.38

Physical Properties

Property code	Value	Unit	Source
gf	-186.60	kJ/mol	Joback Method
hf	-567.45	kJ/mol	Joback Method
hfus	38.28	kJ/mol	Joback Method
hvap	76.48	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.013		Crippen Method
mcvol	251.300	ml/mol	McGowan Method
pc	1628.54	kPa	Joback Method
rinpol	2195.00		NIST Webbook
tb	799.20	K	Joback Method
tc	1006.70	K	Joback Method
tf	455.80	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.28	J/mol×K	799.20	Joback Method
cpg	751.65	J/mol×K	833.78	Joback Method
cpg	765.97	J/mol×K	868.37	Joback Method
cpg	779.27	J/mol×K	902.95	Joback Method
cpg	791.58	J/mol×K	937.53	Joback Method
cpg	802.92	J/mol×K	972.11	Joback Method
cpg	813.34	J/mol×K	1006.70	Joback Method
dvisc	0.0007598	Pa×s	455.80	Joback Method
dvisc	0.0003887	Pa×s	513.03	Joback Method

dvisc	0.0002275	Pa×s	570.27	Joback Method
dvisc	0.0001468	Pa×s	627.50	Joback Method
dvisc	0.0001020	Pa×s	684.73	Joback Method
dvisc	0.0000749	Pa×s	741.97	Joback Method
dvisc	0.0000575	Pa×s	799.20	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=U356686&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