Isophthalic acid, butyl cis-hex-3-enyl ester

Inchi: InChI=1S/C18H24O4/c1-3-5-7-8-13-22-18(20)16-11-9-10-15(14-16)17(19)21-12-6-4-2/h5
InchiKey: QJWBUTMYQPXRQV-ALCCZGGFSA-N
Formula: C18H24O4
SMILES: CCC=CCCOC(=O)c1cccc(C(=O)OCCCC)c1
Mol. weight [g/mol]: 304.38

Physical Properties

Property code	Value	Unit	Source
gf	-184.16	kJ/mol	Joback Method
hf	-562.17	kJ/mol	Joback Method
hfus	41.80	kJ/mol	Joback Method
hvap	76.87	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.157		Crippen Method
mcvol	251.300	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	2246.00		NIST Webbook
rinpol	2246.00		NIST Webbook
tb	799.64	K	Joback Method
tc	1004.52	K	Joback Method
tf	470.80	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.73	J/mol×K	799.64	Joback Method
cpg	801.78	J/mol×K	970.37	Joback Method
cpg	790.48	J/mol×K	936.23	Joback Method
cpg	778.26	J/mol×K	902.08	Joback Method
cpg	765.08	J/mol×K	867.93	Joback Method
cpg	750.91	J/mol×K	833.79	Joback Method
cpg	812.18	J/mol×K	1004.52	Joback Method
dvisc	0.0000626	Pa×s	799.64	Joback Method

dvisc	0.0000803	Pa×s	744.83	Joback Method
dvisc	0.0001070	Pa×s	690.03	Joback Method
dvisc	0.0001500	Pa×s	635.22	Joback Method
dvisc	0.0002241	Pa×s	580.41	Joback Method
dvisc	0.0003640	Pa×s	525.61	Joback Method
dvisc	0.0006620	Pa×s	470.80	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=U356699&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