

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/molxK	799.20	Joback Method
cpg	751.65	J/molxK	833.78	Joback Method
cpg	765.97	J/molxK	868.37	Joback Method
cpg	779.27	J/molxK	902.95	Joback Method
cpg	791.58	J/molxK	937.53	Joback Method
cpg	802.92	J/molxK	972.11	Joback Method
cpg	813.34	J/molxK	1006.70	Joback Method
dvisc	0.0007598	Paxs	455.80	Joback Method
dvisc	0.0003887	Paxs	513.03	Joback Method

dvisc	0.0002275	Paxs	570.27	Joback Method
dvisc	0.0001468	Paxs	627.50	Joback Method
dvisc	0.0001020	Paxs	684.73	Joback Method
dvisc	0.0000749	Paxs	741.97	Joback Method
dvisc	0.0000575	Paxs	799.20	Joback Method

Sources

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/ci9903071
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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