

Phthalic acid, isobutyl trans-dec-3-enyl ester

Inchi:	InChI=1S/C22H32O4/c1-4-5-6-7-8-9-10-13-16-25-21(23)19-14-11-12-15-20(19)22(24)26
InchiKey:	LBEYCBOSHBVHIP-DTQAZKPQSA-N
Formula:	C22H32O4
SMILES:	CCCCCCCCC=COC(=O)c1ccccc1C(=O)OCC(C)C
Mol. weight [g/mol]:	360.49

Physical Properties

Property code	Value	Unit	Source
gf	-152.92	kJ/mol	Joback Method
hf	-650.01	kJ/mol	Joback Method
hfus	48.64	kJ/mol	Joback Method
hvap	85.39	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	5.921		Crippen Method
mcvol	307.660	ml/mol	McGowan Method
pc	1220.85	kPa	Joback Method
rinsol	2491.00		NIST Webbook
tb	890.72	K	Joback Method
tc	1098.22	K	Joback Method
tf	500.88	K	Joback Method
vc	1.181	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.52	J/molxK	890.72	Joback Method
cpg	986.72	J/molxK	925.30	Joback Method
cpg	1001.75	J/molxK	959.89	Joback Method
cpg	1015.64	J/molxK	994.47	Joback Method
cpg	1028.44	J/molxK	1029.05	Joback Method
cpg	1040.19	J/molxK	1063.63	Joback Method
cpg	1050.94	J/molxK	1098.22	Joback Method
dvisc	0.0005015	Paxs	500.88	Joback Method
dvisc	0.0002455	Paxs	565.85	Joback Method

dvisc	0.0001393	Paxs	630.83	Joback Method
dvisc	0.0000878	Paxs	695.80	Joback Method
dvisc	0.0000599	Paxs	760.77	Joback Method
dvisc	0.0000434	Paxs	825.75	Joback Method
dvisc	0.0000330	Paxs	890.72	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=U360499&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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