

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

Inchi:	InChI=1S/C22H32O4/c1-3-5-7-9-10-12-17-26-22(24)20-15-13-14-19(18-20)21(23)25-16-
InchiKey:	OFUQKMMBLLJYKL-VURMDHGXSA-N
Formula:	C22H32O4
SMILES:	CCC=CCCOC(=O)c1cccc(C(=O)OCCCCCCCC)c1
Mol. weight [g/mol]:	360.49

Physical Properties

Property code	Value	Unit	Source
gf	-150.48	kJ/mol	Joback Method
hf	-644.73	kJ/mol	Joback Method
hfus	52.16	kJ/mol	Joback Method
hvap	85.77	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	5.717		Crippen Method
mvol	307.660	ml/mol	McGowan Method
pc	1214.05	kPa	Joback Method
rinpol	2648.00		NIST Webbook
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tb	891.16	K	Joback Method
tc	1097.33	K	Joback Method
tf	515.88	K	Joback Method
vc	1.188	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.03	J/molxK	891.16	Joback Method
cpg	986.16	J/molxK	925.52	Joback Method
cpg	1001.14	J/molxK	959.88	Joback Method
cpg	1015.00	J/molxK	994.25	Joback Method
cpg	1027.80	J/molxK	1028.61	Joback Method
cpg	1039.58	J/molxK	1062.97	Joback Method
cpg	1050.37	J/molxK	1097.33	Joback Method
dvisc	0.0004447	Paxs	515.88	Joback Method

dvisc	0.0002333	Paxs	578.43	Joback Method
dvisc	0.0001388	Paxs	640.97	Joback Method
dvisc	0.0000906	Paxs	703.52	Joback Method
dvisc	0.0000634	Paxs	766.07	Joback Method
dvisc	0.0000468	Paxs	828.61	Joback Method
dvisc	0.0000361	Paxs	891.16	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U356702&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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