

Isophthalic acid, hex-3-yl undecyl ester

Inchi:	InChI=1S/C25H40O4/c1-4-7-8-9-10-11-12-13-14-19-28-24(26)21-17-15-18-22(20-21)25(
InchiKey:	ZZZZMBAHALOCDO-UHFFFAOYSA-N
Formula:	C25H40O4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OC(CC)CCC)c1
Mol. weight [g/mol]:	404.58

Physical Properties

Property code	Value	Unit	Source
gf	-207.88	kJ/mol	Joback Method
hf	-829.15	kJ/mol	Joback Method
hfus	56.21	kJ/mol	Joback Method
hvap	92.11	kJ/mol	Joback Method
log10ws	-8.35		Crippen Method
logp	7.110		Crippen Method
mcvol	354.230	ml/mol	McGowan Method
pc	975.34	kPa	Joback Method
rinpol	2936.00		NIST Webbook
tb	955.20	K	Joback Method
tc	1169.50	K	Joback Method
tf	539.77	K	Joback Method
vc	1.369	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.72	J/molxK	955.20	Joback Method
cpg	1253.77	J/molxK	1133.79	Joback Method
cpg	1242.11	J/molxK	1098.07	Joback Method
cpg	1229.11	J/molxK	1062.35	Joback Method
cpg	1214.75	J/molxK	1026.63	Joback Method
cpg	1198.96	J/molxK	990.92	Joback Method
cpg	1264.15	J/molxK	1169.50	Joback Method
dvisc	0.0000242	Paxs	955.20	Joback Method
dvisc	0.0000320	Paxs	885.96	Joback Method

dvisc	0.0000443	Paxs	816.72	Joback Method
dvisc	0.0000654	Paxs	747.48	Joback Method
dvisc	0.0001043	Paxs	678.25	Joback Method
dvisc	0.0001851	Paxs	609.01	Joback Method
dvisc	0.0003804	Paxs	539.77	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=U356484&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

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