

Isophthalic acid, pentyl undec-2-en-1-yl ester

Inchi:	InChI=1S/C24H36O4/c1-3-5-7-8-9-10-11-12-14-19-28-24(26)22-17-15-16-21(20-22)23(2
InchiKey:	MDIBTHBUUIQCED-WYMLVPIESA-N
Formula:	C24H36O4
SMILES:	CCCCCCCC=CCOC(=O)c1cccc(C(=O)OCCCC)c1
Mol. weight [g/mol]:	388.54

Physical Properties

Property code	Value	Unit	Source
gf	-133.64	kJ/mol	Joback Method
hf	-686.01	kJ/mol	Joback Method
hfus	57.34	kJ/mol	Joback Method
hvap	90.23	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	6.497		Crippen Method
mcvol	335.840	ml/mol	McGowan Method
pc	1066.57	kPa	Joback Method
rinpol	2954.00		NIST Webbook
rinpol	2954.00		NIST Webbook
tb	936.92	K	Joback Method
tc	1148.38	K	Joback Method
tf	538.42	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.52	J/molxK	936.92	Joback Method
cpg	1162.71	J/molxK	1113.14	Joback Method
cpg	1150.76	J/molxK	1077.89	Joback Method
cpg	1137.72	J/molxK	1042.65	Joback Method
cpg	1123.53	J/molxK	1007.41	Joback Method
cpg	1108.15	J/molxK	972.16	Joback Method
cpg	1173.61	J/molxK	1148.38	Joback Method
dvisc	0.0000270	Paxs	936.92	Joback Method

dvisc	0.0000352	Paxs	870.50	Joback Method
dvisc	0.0000480	Paxs	804.09	Joback Method
dvisc	0.0000692	Paxs	737.67	Joback Method
dvisc	0.0001072	Paxs	671.25	Joback Method
dvisc	0.0001828	Paxs	604.84	Joback Method
dvisc	0.0003558	Paxs	538.42	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=U343906&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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