

Isophthalic acid, pent-4-enyl undecyl 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:	ZSFHQILPYXWXJG-UHFFFAOYSA-N
Formula:	C24H36O4
SMILES:	C=CCCCOC(=O)c1cccc(C(=O)OCCCCCCCCCCC)c1
Mol. weight [g/mol]:	388.54

Physical Properties

Property code	Value	Unit	Source
gf	-126.02	kJ/mol	Joback Method
hf	-677.80	kJ/mol	Joback Method
hfus	55.86	kJ/mol	Joback Method
hvap	89.60	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	6.497		Crippen Method
mcvol	335.840	ml/mol	McGowan Method
pc	1059.64	kPa	Joback Method
rinpol	2849.00		NIST Webbook
tb	929.44	K	Joback Method
tc	1138.95	K	Joback Method
tf	541.74	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1090.34	J/molxK	929.44	Joback Method
cpg	1106.90	J/molxK	964.36	Joback Method
cpg	1122.17	J/molxK	999.28	Joback Method
cpg	1136.18	J/molxK	1034.19	Joback Method
cpg	1148.97	J/molxK	1069.11	Joback Method
cpg	1160.59	J/molxK	1104.03	Joback Method
cpg	1171.08	J/molxK	1138.95	Joback Method
dvisc	0.0003970	Paxs	541.74	Joback Method
dvisc	0.0002105	Paxs	606.36	Joback Method

dvisc	0.0001262	Paxs	670.97	Joback Method
dvisc	0.0000827	Paxs	735.59	Joback Method
dvisc	0.0000581	Paxs	800.21	Joback Method
dvisc	0.0000430	Paxs	864.82	Joback Method
dvisc	0.0000332	Paxs	929.44	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356721&Units=SI

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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