

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

Inchi:	InChI=1S/C27H42O4/c1-3-5-7-9-11-12-13-15-17-22-31-27(29)25-20-18-19-24(23-25)26(
InchiKey:	LDTIMBLABZFHGA-BMRADRMJSA-N
Formula:	C27H42O4
SMILES:	CCCCCCCC=CCOC(=O)c1cccc(C(=O)OCCCCCCCC)c1
Mol. weight [g/mol]:	430.62

Physical Properties

Property code	Value	Unit	Source
gf	-108.38	kJ/mol	Joback Method
hf	-747.93	kJ/mol	Joback Method
hfus	65.11	kJ/mol	Joback Method
hvap	96.90	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	7.668		Crippen Method
mvol	378.110	ml/mol	McGowan Method
pc	891.07	kPa	Joback Method
rinpol	3262.00		NIST Webbook
rinpol	3262.00		NIST Webbook
tb	1005.56	K	Joback Method
tc	1232.11	K	Joback Method
tf	572.23	K	Joback Method
vc	1.468	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1277.89	J/molxK	1005.56	Joback Method
cpg	1295.50	J/molxK	1043.32	Joback Method
cpg	1311.64	J/molxK	1081.08	Joback Method
cpg	1326.39	J/molxK	1118.83	Joback Method
cpg	1339.83	J/molxK	1156.59	Joback Method
cpg	1352.04	J/molxK	1194.35	Joback Method
cpg	1363.08	J/molxK	1232.11	Joback Method
dvisc	0.0002485	Paxs	572.23	Joback Method

dvisc	0.0001241	Paxs	644.45	Joback Method
dvisc	0.0000712	Paxs	716.67	Joback Method
dvisc	0.0000453	Paxs	788.89	Joback Method
dvisc	0.0000311	Paxs	861.12	Joback Method
dvisc	0.0000226	Paxs	933.34	Joback Method
dvisc	0.0000172	Paxs	1005.56	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=U343910&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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