

Phthalic acid, trans-hex-3-enyl undecyl ester

Inchi:	InChI=1S/C25H38O4/c1-3-5-7-9-10-11-12-13-17-21-29-25(27)23-19-15-14-18-22(23)24(
InchiKey:	SQTXPSZQBUGJMR-SOFGYWHQSA-N
Formula:	C25H38O4
SMILES:	CCC=CCCOC(=O)c1cccc1C(=O)OCCCCCCCCCCC
Mol. weight [g/mol]:	402.57

Physical Properties

Property code	Value	Unit	Source
gf	-125.22	kJ/mol	Joback Method
hf	-706.65	kJ/mol	Joback Method
hfus	59.93	kJ/mol	Joback Method
hvap	92.45	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	6.887		Crippen Method
mcvol	349.930	ml/mol	McGowan Method
pc	1002.71	kPa	Joback Method
rinsol	2841.00		NIST Webbook
tb	959.80	K	Joback Method
tc	1175.26	K	Joback Method
tf	549.69	K	Joback Method
vc	1.355	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1153.14	J/molxK	959.80	Joback Method
cpg	1170.06	J/molxK	995.71	Joback Method
cpg	1185.67	J/molxK	1031.62	Joback Method
cpg	1200.03	J/molxK	1067.53	Joback Method
cpg	1213.20	J/molxK	1103.44	Joback Method
cpg	1225.23	J/molxK	1139.35	Joback Method
cpg	1236.18	J/molxK	1175.26	Joback Method
dvisc	0.0003167	Paxs	549.69	Joback Method
dvisc	0.0001611	Paxs	618.04	Joback Method

dvisc	0.0000938	Paxs	686.39	Joback Method
dvisc	0.0000602	Paxs	754.74	Joback Method
dvisc	0.0000416	Paxs	823.10	Joback Method
dvisc	0.0000304	Paxs	891.45	Joback Method
dvisc	0.0000233	Paxs	959.80	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=U360489&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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