1,2-Benzenedicarboxylic acid, diundecyl ester

Other names:	1,2-Benzenedicarboxylic acid, 1,2-diundecyl ester
	DUP
	Di-n-undecyl phthalate
	Jayflex DUP
	Jayflex L 11P
	Phthalic acid, diundecyl ester
	diundecyl phthalate
Inchi:	InChI=1S/C30H50O4/c1-3-5-7-9-11-13-15-17-21-25-33-29(31)27-23-19-20-24-28(27)30(
InchiKey:	QQVHEQUEHCEAKS-UHFFFAOYSA-N
Formula:	C30H50O4
SMILES:	CCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCCCCCCCCCC
Mol. weight [g/mol]:	474.72
CAS:	3648-20-2

Physical Properties

Property code	Value	Unit	Source
gf	-163.34	kJ/mol	Joback Method
hf	-927.07	kJ/mol	Joback Method
hfus	72.68	kJ/mol	Joback Method
hvap	103.62	kJ/mol	Joback Method
log10ws	-10.33		Crippen Method
logp	9.062		Crippen Method
mcvol	424.680	ml/mol	McGowan Method
pc	890.00	kPa	Critical Temperatures and Pressures of 12 Phthalates Using the Pulse-Heating Method
tb	1070.04	K	Joback Method
tc	1324.57	K	Joback Method
tf	611.12	K	Joback Method
vc	1.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	1496.84	J/mol×K	1070.04	Joback Method
cpg	1515.88	J/mol×K	1112.46	Joback Method
cpg	1532.83	J/mol×K	1154.88	Joback Method
cpg	1547.78	J/mol×K	1197.31	Joback Method
cpg	1560.83	J/mol×K	1239.73	Joback Method
cpg	1572.09	J/mol×K	1282.15	Joback Method
cpg	1581.64	J/mol×K	1324.57	Joback Method
dvisc	0.0001828	Pa×s	611.12	Joback Method
dvisc	0.0000907	Pa×s	687.61	Joback Method
dvisc	0.0000517	Pa×s	764.09	Joback Method
dvisc	0.0000327	Pa×s	840.58	Joback Method
dvisc	0.0000223	Pa×s	917.07	Joback Method
dvisc	0.0000161	Pa×s	993.55	Joback Method
dvisc	0.0000122	Pa×s	1070.04	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	524.00 ± 1.00	K	0.03	NIST Webbook

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=C3648202&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Critical Temperatures and Pressures of 12 Phthalates Using the Pulse-Heating Method:	https://www.doi.org/10.1021/je060068f

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume