Phthalic acid, 2,2-dimethylpent-3-yl undecyl ester

Inchi: InChI=1S/C26H42O4/c1-6-8-9-10-11-12-13-14-17-20-29-24(27)21-18-15-16-19-22(21)25

InchiKey: SKDDWDFBJPDDRB-UHFFFAOYSA-N

Formula: C26H42O4

SMILES: CCCCCCCCCCCOC(=O)c1ccccc1C(=O)OC(CC)C(C)(C)C

Mol. weight [g/mol]: 418.61

Physical Properties

Property code	Value	Unit	Source
gf	-196.62	kJ/mol	Joback Method
hf	-858.54	kJ/mol	Joback Method
hfus	51.38	kJ/mol	Joback Method
hvap	93.04	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	7.356		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	930.07	kPa	Joback Method
rinpol	3002.00		NIST Webbook
rinpol	3002.00		NIST Webbook
tb	974.85	K	Joback Method
tc	1193.64	K	Joback Method
tf	553.46	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1243.96	J/mol×K	974.85	Joback Method
cpg	1261.44	J/mol×K	1011.31	Joback Method
cpg	1277.49	J/mol×K	1047.78	Joback Method
cpg	1292.20	J/mol×K	1084.24	Joback Method
cpg	1305.62	J/mol×K	1120.71	Joback Method
cpg	1317.83	J/mol×K	1157.17	Joback Method
cpg	1328.91	J/mol×K	1193.64	Joback Method
dvisc	0.0002960	Pa×s	553.46	Joback Method

dvisc	0.0001378	Pa×s	623.69	Joback Method
dvisc	0.0000749	Pa×s	693.92	Joback Method
dvisc	0.0000456	Pa×s	764.15	Joback Method
dvisc	0.0000301	Pa×s	834.39	Joback Method
dvisc	0.0000212	Pa×s	904.62	Joback Method
dvisc	0.0000158	Pa×s	974.85	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=U415534&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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