Phthalic acid, di(dec-2-yl) ester

Other names: 1,2-Benzenedicarboxylic acid, didecan-2-yl ester
Phthalic acid, di(dec-2-yl) ester
Inchi: InChI=1S/C28H46O4/c1-5-7-9-11-13-15-19-23(3)31-27(29)25-21-17-18-22-26(25)28(30)32-24(4)20-16-14-12-10-8-6-2
InchiKey: CZTAPVBKUXXDLY-UHFFFAOYSA-N
Formula: C28H46O4
SMILES: CCCCCCCCC(C)OC(=O)c1ccccc1C(=O)OC(C)CCCCCCCC
Mol. weight [g/mol]: 446.67

Physical Properties

Property code	Value	Unit	Source
hf	-1025.14	kJ/mol	Cheméo Relay (1.0)
hfus	60.46	kJ/mol	Joback Method
hvap	120.11	kJ/mol	Cheméo Relay (1.0)
ie	9.35	eV	Cheméo Relay (1.0)
log10ws	-7.58		Cheméo Relay (1.0)
logp	8.278		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	824.79	kPa	Joback Method
rinpol	2956.00		NIST Webbook
rinpol	2910.00		NIST Webbook
tb	668.50	K	Cheméo Relay (1.0)
tf	276.77	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1370.15	J/mol×K	1023.40	Joback Method
cpg	1388.07	J/mol×K	1062.11	Joback Method
cpg	1404.21	J/mol×K	1100.83	Joback Method
cpg	1418.64	J/mol×K	1139.54	Joback Method
cpg	1431.44	J/mol×K	1178.25	Joback Method
cpg	1442.65	J/mol×K	1216.97	Joback Method
cpg	1452.37	J/mol×K	1255.68	Joback Method
dvisc	0.0002898	Pa×s	558.58	Joback Method

dvisc	0.0001282	Pa×s	636.05	Joback Method
dvisc	0.0000677	Pa×s	713.52	Joback Method
dvisc	0.0000405	Pa×s	790.99	Joback Method
dvisc	0.0000266	Pa×s	868.46	Joback Method
dvisc	0.0000187	Pa×s	945.93	Joback Method
dvisc	0.0000138	Pa×s	1023.40	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28029892&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point