Phthalic acid, dodecyl hept-4-yl ester

Inchi: InChI=1S/C27H44O4/c1-4-7-8-9-10-11-12-13-14-17-22-30-26(28)24-20-15-16-21-25(24)27(29)31-23(18-5-2)19-6-3/h15-16,20-21,23H,4-14,17-19,22H2,1-3H3

InchiKey: RFFHNFMAXNPOGC-UHFFFAOYSA-N

Formula: C27H44O4

SMILES: CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OC(CCC)CCC

Mol. weight [g/mol]: 432.64

Physical Properties

Property code	Value	Unit	Source
gf	-191.04	kJ/mol	Joback Method
hf	-870.43	kJ/mol	Joback Method
hfus	61.39	kJ/mol	Joback Method
hvap	96.56	kJ/mol	Joback Method
log10ws	-9.18		Crippen Method
logp	7.890		Crippen Method
mcvol	382.410	ml/mol	McGowan Method
pc	868.11	kPa	Joback Method
rinpol	2913.00		NIST Webbook
tb	1000.96	K	Joback Method
tc	1226.87	K	Joback Method
tf	562.31	K	Joback Method
vc	1.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1306.77	J/mol×K	1000.96	Joback Method
cpg	1324.54	J/mol×K	1038.61	Joback Method
cpg	1340.65	J/mol×K	1076.26	Joback Method
cpg	1355.17	J/mol×K	1113.92	Joback Method
cpg	1368.14	J/mol×K	1151.57	Joback Method
cpg	1379.63	J/mol×K	1189.22	Joback Method
cpg	1389.70	J/mol×K	1226.87	Joback Method
dvisc	0.0002962	Pa×s	562.31	Joback Method
dvisc	0.0001415	Pa×s	635.42	Joback Method

dvisc	0.0000788	Pa×s	708.53	Joback Method
dvisc	0.0000489	Pa×s	781.63	Joback Method
dvisc	0.0000330	Pa×s	854.74	Joback Method
dvisc	0.0000236	Pa×s	927.85	Joback Method
dvisc	0.0000178	Pa×s	1000.96	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=U356793&Units=SI

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