Isophthalic acid, 2-methylprop-2-en-1-yl pentadecyl ester

Inchi: InChI=1S/C27H42O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-20-30-26(28)24-18-17-19-25

InchiKey: WVKFYGCJGIHUOM-UHFFFAOYSA-N

Formula: C27H42O4

SMILES: C=C(C)COC(=O)c1cccc(C(=O)OCCCCCCCCCCCCCCC)c1

Mol. weight [g/mol]: 430.62

Physical Properties

Property code	Value	Unit	Source
gf	-109.31	kJ/mol	Joback Method
hf	-749.51	kJ/mol	Joback Method
hfus	62.32	kJ/mol	Joback Method
hvap	96.36	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	7.668		Crippen Method
mcvol	378.110	ml/mol	McGowan Method
pc	888.41	kPa	Joback Method
rinpol	3238.00		NIST Webbook
rinpol	3238.00		NIST Webbook
tb	997.96	K	Joback Method
tc	1222.59	K	Joback Method
tf	561.59	K	Joback Method
vc	1.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1275.98	J/mol×K	997.96	Joback Method
cpg	1293.43	J/mol×K	1035.40	Joback Method
cpg	1309.34	J/mol×K	1072.84	Joback Method
cpg	1323.78	J/mol×K	1110.27	Joback Method
cpg	1336.82	J/mol×K	1147.71	Joback Method
cpg	1348.52	J/mol×K	1185.15	Joback Method
cpg	1358.93	J/mol×K	1222.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343956&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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