Isophthalic acid, heptadecyl 1-propylbutyl ester

Inchi: InChI=1S/C32H54O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-26-35-31(33)28-24-

InchiKey: XTFDLYNRLRYKEF-UHFFFAOYSA-N

Formula: C32H54O4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(CCC)CCC)c1

Mol. weight [g/mol]: 502.77

Physical Properties

Property code	Value	Unit	Source
gf	-148.94	kJ/mol	Joback Method
hf	-973.63	kJ/mol	Joback Method
hfus	74.34	kJ/mol	Joback Method
hvap	107.69	kJ/mol	Joback Method
log10ws	-11.28		Crippen Method
logp	9.840		Crippen Method
mcvol	452.860	ml/mol	McGowan Method
pc	666.32	kPa	Joback Method
rinpol	3510.00		NIST Webbook
rinpol	3510.00		NIST Webbook
tb	1115.36	K	Joback Method
tc	1392.23	K	Joback Method
tf	618.66	K	Joback Method
vc	1.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1625.12	J/mol×K	1115.36	Joback Method
cpg	1644.77	J/mol×K	1161.51	Joback Method
cpg	1661.93	J/mol×K	1207.65	Joback Method
cpg	1676.76	J/mol×K	1253.80	Joback Method
cpg	1689.40	J/mol×K	1299.94	Joback Method
cpg	1699.99	J/mol×K	1346.09	Joback Method
cpg	1708.67	J/mol×K	1392.23	Joback Method
dvisc	0.0001518	Pa×s	618.66	Joback Method

dvisc	0.0000697	Pa×s	701.44	Joback Method
dvisc	0.0000377	Pa×s	784.23	Joback Method
dvisc	0.0000230	Pa×s	867.01	Joback Method
dvisc	0.0000152	Pa×s	949.79	Joback Method
dvisc	0.0000108	Pa×s	1032.58	Joback Method
dvisc	0.0000081	Pa×s	1115.36	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=U356412&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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