Isophthalic acid, 4-methylpent-2-yl octadecyl ester

Inchi: InChI=1S/C32H54O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-35-31(33)29-2

InchiKey: SKNCLPFHVISLAJ-UHFFFAOYSA-N

Formula: C32H54O4

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)CC(C)C)c1

Mol. weight [g/mol]: 502.77

Physical Properties

Property code	Value	Unit	Source
gf	-151.38	kJ/mol	Joback Method
hf	-978.91	kJ/mol	Joback Method
hfus	70.82	kJ/mol	Joback Method
hvap	107.30	kJ/mol	Joback Method
log10ws	-11.04		Crippen Method
logp	9.696		Crippen Method
mcvol	452.860	ml/mol	McGowan Method
pc	669.08	kPa	Joback Method
rinpol	3525.00		NIST Webbook
tb	1114.92	K	Joback Method
tc	1388.61	K	Joback Method
tf	603.66	K	Joback Method
vc	1.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1625.17	J/mol×K	1114.92	Joback Method
cpg	1644.48	J/mol×K	1160.53	Joback Method
cpg	1661.34	J/mol×K	1206.15	Joback Method
cpg	1675.89	J/mol×K	1251.76	Joback Method
cpg	1688.27	J/mol×K	1297.38	Joback Method
cpg	1698.62	J/mol×K	1342.99	Joback Method
cpg	1707.08	J/mol×K	1388.61	Joback Method
dvisc	0.0001665	Pa×s	603.66	Joback Method
dvisc	0.0000716	Pa×s	688.87	Joback Method

dvisc	0.0000371	Pa×s	774.08	Joback Method
dvisc	0.0000219	Pa×s	859.29	Joback Method
dvisc	0.0000142	Pa×s	944.50	Joback Method
dvisc	0.0000099	Pa×s	1029.71	Joback Method
dvisc	0.0000073	Pa×s	1114.92	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=U356455&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

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