

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:	CCCCCCCCCCCCCCCCCOC(=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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000371	Paxs	774.08	Joback Method
dvisc	0.0000219	Paxs	859.29	Joback Method
dvisc	0.0000142	Paxs	944.50	Joback Method
dvisc	0.0000099	Paxs	1029.71	Joback Method
dvisc	0.0000073	Paxs	1114.92	Joback Method

Sources

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

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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