

Phthalic acid, hexadecyl 2-propylpentyl ester

Inchi:	InChI=1S/C32H54O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-21-26-35-31(33)29-24-19-
InchiKey:	GHIUKKNNGVQMQUI-UHFFFAOYSA-N
Formula:	C32H54O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCC(CCC)CCC
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	-10.92		Crippen Method
logp	9.698		Crippen Method
mvol	452.860	ml/mol	McGowan Method
pc	666.32	kPa	Joback Method
rinpol	3443.00		NIST Webbook
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tb	1115.36	K	Joback Method
tc	1392.23	K	Joback Method
tf	618.66	K	Joback Method
vc	1.762	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1625.12	J/molxK	1115.36	Joback Method
cpg	1699.99	J/molxK	1346.09	Joback Method
cpg	1689.40	J/molxK	1299.94	Joback Method
cpg	1676.76	J/molxK	1253.80	Joback Method
cpg	1661.93	J/molxK	1207.65	Joback Method
cpg	1644.77	J/molxK	1161.51	Joback Method
cpg	1708.67	J/molxK	1392.23	Joback Method
dvisc	0.0000081	Paxs	1115.36	Joback Method

dvisc	0.0000108	Paxs	1032.58	Joback Method
dvisc	0.0000152	Paxs	949.79	Joback Method
dvisc	0.0000230	Paxs	867.01	Joback Method
dvisc	0.0000377	Paxs	784.23	Joback Method
dvisc	0.0000697	Paxs	701.44	Joback Method
dvisc	0.0001518	Paxs	618.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377932&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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