

Phthalic acid, octadecyl trans-hex-3-enyl ester

Inchi:	InChI=1S/C32H52O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-20-24-28-36-32(34)30-
InchiKey:	YAPKMXPAPDIWEF-SOFGYWHQSA-N
Formula:	C32H52O4
SMILES:	CCC=CCCOC(=O)c1cccc1C(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	500.75

Physical Properties

Property code	Value	Unit	Source
gf	-66.28	kJ/mol	Joback Method
hf	-851.13	kJ/mol	Joback Method
hfus	78.06	kJ/mol	Joback Method
hvap	108.03	kJ/mol	Joback Method
log10ws	-11.02		Crippen Method
logp	9.618		Crippen Method
mvol	448.560	ml/mol	McGowan Method
pc	681.71	kPa	Joback Method
rinpol	3563.00		NIST Webbook
tb	1119.96	K	Joback Method
tc	1395.96	K	Joback Method
tf	628.58	K	Joback Method
vc	1.748	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1596.66	J/molxK	1119.96	Joback Method
cpg	1678.25	J/molxK	1349.96	Joback Method
cpg	1665.42	J/molxK	1303.96	Joback Method
cpg	1651.01	J/molxK	1257.96	Joback Method
cpg	1634.86	J/molxK	1211.96	Joback Method
cpg	1616.80	J/molxK	1165.96	Joback Method
cpg	1689.69	J/molxK	1395.96	Joback Method
dvisc	0.0000078	Paxs	1119.96	Joback Method
dvisc	0.0000104	Paxs	1038.06	Joback Method

dvisc	0.0000145	Paxs	956.17	Joback Method
dvisc	0.0000215	Paxs	874.27	Joback Method
dvisc	0.0000346	Paxs	792.37	Joback Method
dvisc	0.0000620	Paxs	710.48	Joback Method
dvisc	0.0001296	Paxs	628.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360496&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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