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

Inchi: InChI=1S/C30H48O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-22-26-34-30(32)28-24-20-
InchiKey: NIWQTKYMCPLYOK-SOFGYWHQSA-N
Formula: C30H48O4
SMILES: CCC=CCCOC(=O)c1ccccc1C(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 472.70

Physical Properties

Property code	Value	Unit	Source
gf	-83.12	kJ/mol	Joback Method
hf	-809.85	kJ/mol	Joback Method
hfus	72.88	kJ/mol	Joback Method
hvap	103.58	kJ/mol	Joback Method
log10ws	-10.18		Crippen Method
logp	8.838		Crippen Method
mcvol	420.380	ml/mol	McGowan Method
pc	755.57	kPa	Joback Method
rinpol	3349.00		NIST Webbook
rinpol	3349.00		NIST Webbook
tb	1074.20	K	Joback Method
tc	1326.23	K	Joback Method
tf	606.04	K	Joback Method
vc	1.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1468.16	J/mol×K	1074.20	Joback Method
cpg	1546.28	J/mol×K	1284.22	Joback Method
cpg	1533.75	J/mol×K	1242.22	Joback Method
cpg	1519.79	J/mol×K	1200.21	Joback Method
cpg	1504.29	J/mol×K	1158.21	Joback Method
cpg	1487.11	J/mol×K	1116.20	Joback Method
cpg	1557.50	J/mol×K	1326.23	Joback Method
dvisc	0.0000108	Pa×s	1074.20	Joback Method

dvisc	0.0000143	Pa×s	996.17	Joback Method
dvisc	0.0000198	Pa×s	918.15	Joback Method
dvisc	0.0000291	Pa×s	840.12	Joback Method
dvisc	0.0000464	Pa×s	762.09	Joback Method
dvisc	0.0000824	Pa×s	684.07	Joback Method
dvisc	0.0001694	Pa×s	606.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360494&Units=SI
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

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