Phthalic acid, heptadecyl pent-4-enyl ester

Inchi: InChI=1S/C30H48O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-22-26-34-30(32)28-24-2
InchiKey: QZSTXNJFGGKDMZ-UHFFFAOYSA-N
Formula: C30H48O4
SMILES: C=CCCCOC(=O)c1ccccc1C(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 472.70

Physical Properties

Property code	Value	Unit	Source
gf	-75.50	kJ/mol	Joback Method
hf	-801.64	kJ/mol	Joback Method
hfus	71.40	kJ/mol	Joback Method
hvap	102.95	kJ/mol	Joback Method
log10ws	-10.18		Crippen Method
logp	8.838		Crippen Method
mcvol	420.380	ml/mol	McGowan Method
pc	751.43	kPa	Joback Method
rinpol	3361.00		NIST Webbook
rinpol	3361.00		NIST Webbook
tb	1066.72	K	Joback Method
tc	1317.87	K	Joback Method
tf	609.36	K	Joback Method
vc	1.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1465.97	J/mol×K	1066.72	Joback Method
cpg	1484.60	J/mol×K	1108.58	Joback Method
cpg	1501.31	J/mol×K	1150.44	Joback Method
cpg	1516.19	J/mol×K	1192.29	Joback Method
cpg	1529.35	J/mol×K	1234.15	Joback Method
cpg	1540.89	J/mol×K	1276.01	Joback Method
cpg	1550.92	J/mol×K	1317.87	Joback Method
dvisc	0.0001911	Pa×s	609.36	Joback Method

dvisc	0.0000957	Pa×s	685.59	Joback Method
dvisc	0.0000551	Pa×s	761.81	Joback Method
dvisc	0.0000350	Pa×s	838.04	Joback Method
dvisc	0.0000240	Pa×s	914.27	Joback Method
dvisc	0.0000175	Pa×s	990.49	Joback Method
dvisc	0.0000133	Pa×s	1066.72	Joback Method

Sources

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=U360476&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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