Phthalic acid, pentadecyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C31H52O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-20-23-34-29(32)27-21-18-19-

InchiKey: NXOQIOKWSWIEMS-UHFFFAOYSA-N

Formula: C31H52O4

SMILES: CCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCC(C)CC(C)(C)C

Mol. weight [g/mol]: 488.74

Physical Properties

Property code	Value	Unit	Source
gf	-154.52	kJ/mol	Joback Method
hf	-961.74	kJ/mol	Joback Method
hfus	64.34	kJ/mol	Joback Method
hvap	104.17	kJ/mol	Joback Method
log10ws	-10.26		Crippen Method
logp	9.164		Crippen Method
mcvol	438.770	ml/mol	McGowan Method
pc	707.71	kPa	Joback Method
rinpol	3279.00		NIST Webbook
tb	1089.25	K	Joback Method
tc	1345.31	K	Joback Method
tf	609.81	K	Joback Method
vc	1.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1561.14	J/mol×K	1089.25	Joback Method
cpg	1640.09	J/mol×K	1302.63	Joback Method
cpg	1627.50	J/mol×K	1259.96	Joback Method
cpg	1613.45	J/mol×K	1217.28	Joback Method
cpg	1597.80	J/mol×K	1174.60	Joback Method
cpg	1580.41	J/mol×K	1131.93	Joback Method
cpg	1651.36	J/mol×K	1345.31	Joback Method
dvisc	0.0000070	Pa×s	1089.25	Joback Method
dvisc	0.0000095	Pa×s	1009.34	Joback Method

dvisc	0.0000136	Pa×s	929.44	Joback Method
dvisc	0.0000209	Pa×s	849.53	Joback Method
dvisc	0.0000350	Pa×s	769.62	Joback Method
dvisc	0.0000662	Pa×s	689.72	Joback Method
dvisc	0.0001477	Pa×s	609.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377781&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

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