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

Inchi: InChI=1S/C32H54O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-21-24-35-30(33)28-22-19-

InchiKey: QNGDPTOSQFDMBS-UHFFFAOYSA-N

Formula: C32H54O4

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

Mol. weight [g/mol]: 502.77

Physical Properties

Property code	Value	Unit	Source
gf	-146.10	kJ/mol	Joback Method
hf	-982.38	kJ/mol	Joback Method
hfus	66.93	kJ/mol	Joback Method
hvap	106.39	kJ/mol	Joback Method
log10ws	-10.68		Crippen Method
logp	9.554		Crippen Method
mcvol	452.860	ml/mol	McGowan Method
pc	672.90	kPa	Joback Method
rinpol	3381.00		NIST Webbook
rinpol	3381.00		NIST Webbook
tb	1112.13	K	Joback Method
tc	1379.62	K	Joback Method
tf	621.08	K	Joback Method
vc	1.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1625.54	J/mol×K	1112.13	Joback Method
cpg	1706.04	J/mol×K	1335.04	Joback Method
cpg	1693.31	J/mol×K	1290.46	Joback Method
cpg	1679.06	J/mol×K	1245.87	Joback Method
cpg	1663.13	J/mol×K	1201.29	Joback Method
cpg	1645.34	J/mol×K	1156.71	Joback Method
cpg	1717.42	J/mol×K	1379.62	Joback Method
dvisc	0.0000059	Pa×s	1112.13	Joback Method

dvisc	0.0000081	Pa×s	1030.29	Joback Method
dvisc	0.0000116	Pa×s	948.45	Joback Method
dvisc	0.0000178	Pa×s	866.61	Joback Method
dvisc	0.0000299	Pa×s	784.76	Joback Method
dvisc	0.0000568	Pa×s	702.92	Joback Method
dvisc	0.0001278	Pa×s	621.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377782&Units=SI

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