Isophthalic acid, hexadecyl 4-methylpent-2-yl ester

Inchi: InChI=1S/C30H50O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-33-29(31)27-20-19-2

InchiKey: ZHDORUBQAQSLCT-UHFFFAOYSA-N

Formula: C30H50O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)CC(C)C)c1

Mol. weight [g/mol]: 474.72

Physical Properties

Property code	Value	Unit	Source
gf	-168.22	kJ/mol	Joback Method
hf	-937.63	kJ/mol	Joback Method
hfus	65.64	kJ/mol	Joback Method
hvap	102.85	kJ/mol	Joback Method
log10ws	-10.20		Crippen Method
logp	8.916		Crippen Method
mcvol	424.680	ml/mol	McGowan Method
pc	740.84	kPa	Joback Method
rinpol	3313.00		NIST Webbook
rinpol	3313.00		NIST Webbook
tb	1069.16	K	Joback Method
tc	1319.32	K	Joback Method
tf	581.12	K	Joback Method
vc	1.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1497.17	J/mol×K	1069.16	Joback Method
cpg	1515.72	J/mol×K	1110.85	Joback Method
cpg	1532.20	J/mol×K	1152.55	Joback Method
cpg	1546.71	J/mol×K	1194.24	Joback Method
cpg	1559.34	J/mol×K	1235.93	Joback Method
cpg	1570.20	J/mol×K	1277.62	Joback Method
cpg	1579.37	J/mol×K	1319.32	Joback Method
dvisc	0.0002206	Pa×s	581.12	Joback Method

dvisc	0.0000962	Pa×s	662.46	Joback Method
dvisc	0.0000503	Pa×s	743.80	Joback Method
dvisc	0.0000299	Pa×s	825.14	Joback Method
dvisc	0.0000195	Pa×s	906.48	Joback Method
dvisc	0.0000136	Pa×s	987.82	Joback Method
dvisc	0.0000101	Pa×s	1069.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356453&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