Isophthalic acid, cyclopentylmethyl hexadecyl ester

Inchi: InChI=1S/C30H48O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-23-33-29(31)27-21-18-22-28

InchiKey: HSMQLJVFGDINKE-UHFFFAOYSA-N

Formula: C30H48O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC2CCCC2)c1

Mol. weight [g/mol]: 472.70

Physical Properties

Property code	Value	Unit	Source
gf	-126.79	kJ/mol	Joback Method
hf	-866.59	kJ/mol	Joback Method
hfus	66.62	kJ/mol	Joback Method
hvap	103.88	kJ/mol	Joback Method
log10ws	-9.98		Crippen Method
logp	8.672		Crippen Method
mcvol	413.820	ml/mol	McGowan Method
pc	811.68	kPa	Joback Method
rinpol	3740.00		NIST Webbook
rinpol	3740.00		NIST Webbook
tb	1085.32	K	Joback Method
tc	1334.08	K	Joback Method
tf	622.02	K	Joback Method
vc	1.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1486.81	J/mol×K	1085.32	Joback Method
cpg	1504.48	J/mol×K	1126.78	Joback Method
cpg	1520.20	J/mol×K	1168.24	Joback Method
cpg	1534.08	J/mol×K	1209.70	Joback Method
cpg	1546.24	J/mol×K	1251.16	Joback Method
cpg	1556.77	J/mol×K	1292.62	Joback Method
cpg	1565.79	J/mol×K	1334.08	Joback Method
dvisc	0.0002508	Pa×s	622.02	Joback Method

dvisc	0.0001285	Pa×s	699.24	Joback Method
dvisc	0.0000752	Pa×s	776.45	Joback Method
dvisc	0.0000485	Pa×s	853.67	Joback Method
dvisc	0.0000337	Pa×s	930.89	Joback Method
dvisc	0.0000247	Pa×s	1008.10	Joback Method
dvisc	0.0000189	Pa×s	1085.32	Joback Method

Sources

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=R475628&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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