Isophthalic acid, 3-methylpentyl pentadecyl ester

Inchi: InChI=1S/C29H48O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-22-32-28(30)26-19-18-20-2

InchiKey: CIFRHSBZAZSWFD-UHFFFAOYSA-N

Formula: C29H48O4

SMILES: CCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCC(C)CC)c1

Mol. weight [g/mol]: 460.69

Physical Properties

Property code	Value	Unit	Source
gf	-174.20	kJ/mol	Joback Method
hf	-911.71	kJ/mol	Joback Method
hfus	66.57	kJ/mol	Joback Method
hvap	101.01	kJ/mol	Joback Method
log10ws	-9.67		Crippen Method
logp	8.528		Crippen Method
mcvol	410.590	ml/mol	McGowan Method
pc	777.64	kPa	Joback Method
rinpol	3347.00		NIST Webbook
tb	1046.72	K	Joback Method
tc	1288.88	K	Joback Method
tf	584.85	K	Joback Method
vc	1.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.30	J/mol×K	1046.72	Joback Method
cpg	1451.71	J/mol×K	1087.08	Joback Method
cpg	1468.21	J/mol×K	1127.44	Joback Method
cpg	1482.86	J/mol×K	1167.80	Joback Method
cpg	1495.77	J/mol×K	1208.16	Joback Method
cpg	1507.00	J/mol×K	1248.52	Joback Method
cpg	1516.63	J/mol×K	1288.88	Joback Method
dvisc	0.0002283	Pa×s	584.85	Joback Method
dvisc	0.0001073	Pa×s	661.83	Joback Method

dvisc	0.0000590	Pa×s	738.81	Joback Method
dvisc	0.0000363	Pa×s	815.78	Joback Method
dvisc	0.0000243	Pa×s	892.76	Joback Method
dvisc	0.0000173	Pa×s	969.74	Joback Method
dvisc	0.0000130	Pa×s	1046.72	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=U356159&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

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