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

Inchi: InChI=1S/C29H48O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-21-32-28(30)26-19-18-20-2

InchiKey: IQGURAZSQJFYRN-UHFFFAOYSA-N

Formula: C29H48O4

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

Mol. weight [g/mol]: 460.69

Physical Properties

Property code	Value	Unit	Source
gf	-176.64	kJ/mol	Joback Method
hf	-916.99	kJ/mol	Joback Method
hfus	63.05	kJ/mol	Joback Method
hvap	100.62	kJ/mol	Joback Method
log10ws	-9.78		Crippen Method
logp	8.526		Crippen Method
mcvol	410.590	ml/mol	McGowan Method
pc	781.12	kPa	Joback Method
rinpol	3209.00		NIST Webbook
rinpol	3209.00		NIST Webbook
tb	1046.28	K	Joback Method
tc	1286.84	K	Joback Method
tf	569.85	K	Joback Method
vc	1.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.52	J/mol×K	1046.28	Joback Method
cpg	1451.74	J/mol×K	1086.37	Joback Method
cpg	1468.04	J/mol×K	1126.47	Joback Method
cpg	1482.52	J/mol×K	1166.56	Joback Method
cpg	1495.24	J/mol×K	1206.65	Joback Method
cpg	1506.29	J/mol×K	1246.75	Joback Method
cpg	1515.75	J/mol×K	1286.84	Joback Method
dvisc	0.0002531	Pa×s	569.85	Joback Method

dvisc	0.0001111	Pa×s	649.25	Joback Method
dvisc	0.0000584	Pa×s	728.66	Joback Method
dvisc	0.0000348	Pa×s	808.06	Joback Method
dvisc	0.0000228	Pa×s	887.47	Joback Method
dvisc	0.0000160	Pa×s	966.88	Joback Method
dvisc	0.0000118	Pa×s	1046.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356452&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

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