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

Inchi: InChI=1S/C25H40O4/c1-5-6-7-8-9-10-11-12-13-17-28-24(26)22-15-14-16-23(19-22)25(2

InchiKey: XNKKYWIMQVRBEH-UHFFFAOYSA-N

Formula: C25H40O4

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

Mol. weight [g/mol]: 404.58

Physical Properties

Property code	Value	Unit	Source
gf	-210.32	kJ/mol	Joback Method
hf	-834.43	kJ/mol	Joback Method
hfus	52.69	kJ/mol	Joback Method
hvap	91.72	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	6.966		Crippen Method
mcvol	354.230	ml/mol	McGowan Method
pc	980.23	kPa	Joback Method
rinpol	2796.00		NIST Webbook
tb	954.76	K	Joback Method
tc	1169.19	K	Joback Method
tf	524.77	K	Joback Method
vc	1.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1182.11	J/mol×K	954.76	Joback Method
cpg	1253.86	J/mol×K	1133.45	Joback Method
cpg	1242.28	J/mol×K	1097.71	Joback Method
cpg	1229.37	J/mol×K	1061.98	Joback Method
cpg	1215.06	J/mol×K	1026.24	Joback Method
cpg	1199.33	J/mol×K	990.50	Joback Method
cpg	1264.13	J/mol×K	1169.19	Joback Method
dvisc	0.0000220	Pa×s	954.76	Joback Method
dvisc	0.0000295	Pa×s	883.09	Joback Method

dvisc	0.0000418	Pa×s	811.43	Joback Method
dvisc	0.0000631	Pa×s	739.76	Joback Method
dvisc	0.0001042	Pa×s	668.10	Joback Method
dvisc	0.0001941	Pa×s	596.43	Joback Method
dvisc	0.0004286	Pa×s	524.77	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=U356448&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