

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

Inchi:	InChI=1S/C27H44O4/c1-5-6-7-8-9-10-11-12-13-14-15-19-30-26(28)24-17-16-18-25(21-2
InchiKey:	SLSVRWRHHNUIAN-UHFFFAOYSA-N
Formula:	C27H44O4
SMILES:	CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)CC(C)C)c1
Mol. weight [g/mol]:	432.64

Physical Properties

Property code	Value	Unit	Source
gf	-193.48	kJ/mol	Joback Method
hf	-875.71	kJ/mol	Joback Method
hfus	57.87	kJ/mol	Joback Method
hvap	96.17	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	7.746		Crippen Method
mvol	382.410	ml/mol	McGowan Method
pc	872.22	kPa	Joback Method
rinpol	3000.00		NIST Webbook
tb	1000.52	K	Joback Method
tc	1225.74	K	Joback Method
tf	547.31	K	Joback Method
vc	1.476	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1307.09	J/molxK	1000.52	Joback Method
cpg	1324.74	J/molxK	1038.06	Joback Method
cpg	1340.74	J/molxK	1075.59	Joback Method
cpg	1355.13	J/molxK	1113.13	Joback Method
cpg	1367.98	J/molxK	1150.67	Joback Method
cpg	1379.34	J/molxK	1188.20	Joback Method
cpg	1389.27	J/molxK	1225.74	Joback Method
dvisc	0.0003310	Paxs	547.31	Joback Method
dvisc	0.0001475	Paxs	622.84	Joback Method

dvisc	0.0000783	Paxs	698.38	Joback Method
dvisc	0.0000470	Paxs	773.91	Joback Method
dvisc	0.0000309	Paxs	849.45	Joback Method
dvisc	0.0000218	Paxs	924.99	Joback Method
dvisc	0.0000162	Paxs	1000.52	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U356450&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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