Isophthalic acid, 2-methylprop-2-en-1-yl propyl ester

Inchi: InChI=1S/C15H18O4/c1-4-8-18-14(16)12-6-5-7-13(9-12)15(17)19-10-11(2)3/h5-7,9H,2,4

InchiKey: XQXFTKNDZPADHS-UHFFFAOYSA-N

Formula: C15H18O4

SMILES: C=C(C)COC(=O)c1cccc(C(=O)OCCC)c1

Mol. weight [g/mol]: 262.30

Physical Properties

Property code	Value	Unit	Source
gf	-210.35	kJ/mol	Joback Method
hf	-501.83	kJ/mol	Joback Method
hfus	31.24	kJ/mol	Joback Method
hvap	69.64	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	2.986		Crippen Method
mcvol	209.030	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
rinpol	1979.00		NIST Webbook
tb	723.40	K	Joback Method
tc	932.99	K	Joback Method
tf	426.35	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.94	J/mol×K	723.40	Joback Method
cpg	583.34	J/mol×K	758.33	Joback Method
cpg	596.79	J/mol×K	793.26	Joback Method
cpg	609.31	J/mol×K	828.20	Joback Method
cpg	620.92	J/mol×K	863.13	Joback Method
cpg	631.63	J/mol×K	898.06	Joback Method
cpg	641.45	J/mol×K	932.99	Joback Method

Sources

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=U343945&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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