Isophthalic acid, di(2-methylprop-2-en-1-yl) ester

Inchi: InChI=1S/C16H18O4/c1-11(2)9-19-15(17)13-6-5-7-14(8-13)16(18)20-10-12(3)4/h5-8H,1,

InchiKey: WUXYABHDDLIPKK-UHFFFAOYSA-N

Formula: C16H18O4

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

Mol. weight [g/mol]: 274.31

Physical Properties

Property code	Value	Unit	Source
gf	-122.64	kJ/mol	Joback Method
hf	-406.83	kJ/mol	Joback Method
hfus	31.24	kJ/mol	Joback Method
hvap	71.28	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.152		Crippen Method
mcvol	218.820	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2056.00		NIST Webbook
rinpol	2056.00		NIST Webbook
tb	742.84	K	Joback Method
tc	956.03	K	Joback Method
tf	421.90	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.94	J/mol×K	742.84	Joback Method
cpg	612.32	J/mol×K	778.37	Joback Method
cpg	625.71	J/mol×K	813.90	Joback Method
cpg	638.13	J/mol×K	849.43	Joback Method
cpg	649.63	J/mol×K	884.97	Joback Method
cpg	660.20	J/mol×K	920.50	Joback Method
cpg	669.89	J/mol×K	956.03	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=U343958&Units=SI

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