Isophthalic acid, di(3-methylbut-2-en-1-yl) ester

Inchi: InChI=1S/C18H22O4/c1-13(2)8-10-21-17(19)15-6-5-7-16(12-15)18(20)22-11-9-14(3)4/h5

InchiKey: GDWIJHRQXDVRPC-UHFFFAOYSA-N

Formula: C18H22O4

SMILES: CC(C)=CCOC(=O)c1cccc(C(=O)OCC=C(C)C)c1

Mol. weight [g/mol]: 302.36

Physical Properties

Property code	Value	Unit	Source
gf	-121.04	kJ/mol	Joback Method
hf	-464.53	kJ/mol	Joback Method
hfus	39.39	kJ/mol	Joback Method
hvap	76.99	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	3.933		Crippen Method
mcvol	247.000	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
rinpol	2373.00		NIST Webbook
rinpol	2373.00		NIST Webbook
tb	803.56	K	Joback Method
tc	1019.04	K	Joback Method
tf	437.80	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.28	J/mol×K	803.56	Joback Method
cpg	724.31	J/mol×K	839.47	Joback Method
cpg	738.31	J/mol×K	875.39	Joback Method
cpg	751.35	J/mol×K	911.30	Joback Method
cpg	763.48	J/mol×K	947.21	Joback Method
cpg	774.73	J/mol×K	983.12	Joback Method
cpg	785.16	J/mol×K	1019.04	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=U343943&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