Phthalic acid, isobutyl 3-methylbut-3-enyl ester

Inchi: InChI=1S/C17H22O4/c1-12(2)9-10-20-16(18)14-7-5-6-8-15(14)17(19)21-11-13(3)4/h5-8,

InchiKey: WAOQJPNGIFSUSC-UHFFFAOYSA-N

Formula: C17H22O4

SMILES: C=C(C)CCOC(=O)c1ccccc1C(=O)OCC(C)C

Mol. weight [g/mol]: 290.35

Physical Properties

Property code	Value	Unit	Source
gf	-195.95	kJ/mol	Joback Method
hf	-548.39	kJ/mol	Joback Method
hfus	32.90	kJ/mol	Joback Method
hvap	73.71	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.622		Crippen Method
mcvol	237.210	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	1998.00		NIST Webbook
tb	768.72	K	Joback Method
tc	976.97	K	Joback Method
tf	433.89	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.94	J/mol×K	768.72	Joback Method
cpg	694.22	J/mol×K	803.43	Joback Method
cpg	708.46	J/mol×K	838.14	Joback Method
cpg	721.66	J/mol×K	872.84	Joback Method
cpg	733.86	J/mol×K	907.55	Joback Method
cpg	745.07	J/mol×K	942.26	Joback Method
cpg	755.32	J/mol×K	976.97	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=U357101&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