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

Inchi: InChI=1S/C17H22O4/c1-4-5-11-20-16(18)14-8-6-7-9-15(14)17(19)21-12-10-13(2)3/h6-9H
InchiKey: ARESCACWSBZMSC-UHFFFAOYSA-N
Formula: C17H22O4
SMILES: C=C(C)CCOC(=O)c1ccccc1C(=O)OCCCC
Mol. weight [g/mol]: 290.35

Physical Properties

Property code	Value	Unit	Source
gf	-193.51	kJ/mol	Joback Method
hf	-543.11	kJ/mol	Joback Method
hfus	36.42	kJ/mol	Joback Method
hvap	74.10	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.766		Crippen Method
mcvol	237.210	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
rinpol	2048.00		NIST Webbook
tb	769.16	K	Joback Method
tc	974.46	K	Joback Method
tf	448.89	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.39	J/mol×K	769.16	Joback Method
cpg	693.45	J/mol×K	803.38	Joback Method
cpg	707.50	J/mol×K	837.59	Joback Method
cpg	720.57	J/mol×K	871.81	Joback Method
cpg	732.66	J/mol×K	906.03	Joback Method
cpg	743.81	J/mol×K	940.25	Joback Method
cpg	754.03	J/mol×K	974.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357102&Units=SI
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

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