Bis(3-methylbut-3-enyl) phthalate

Other names: 1,2-Benzenedicarboxylic acid, bis(3-methylbut-3-enyl) ester
Bis(3-methylbut-3-enyl)-1,2-benzenedicarboxylate
Phthalic acid, di(3-methylbut-3-enyl) ester
Inchi: InChI=1S/C18H22O4/c1-13(2)9-11-21-17(19)15-7-5-6-8-16(15)18(20)22-12-10-14(3)4/h5
InchiKey: PKKCFZFIVBCZMZ-UHFFFAOYSA-N
Formula: C18H22O4
SMILES: C=C(C)CCOC(=O)c1ccccc1C(=O)OCCC(=C)C
Mol. weight [g/mol]: 302.36
CAS: 22711-53-1

Physical Properties

Property code	Value	Unit	Source
gf	-105.80	kJ/mol	Joback Method
hf	-448.11	kJ/mol	Joback Method
hfus	36.42	kJ/mol	Joback Method
hvap	75.73	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	3.933		Crippen Method
mcvol	247.000	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
rinpol	2116.00		NIST Webbook
rinpol	2116.00		NIST Webbook
rinpol	2118.00		NIST Webbook
tb	788.60	K	Joback Method
tc	997.40	K	Joback Method
tf	444.44	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.30	J/mol×K	788.60	Joback Method
cpg	723.27	J/mol×K	823.40	Joback Method
cpg	737.21	J/mol×K	858.20	Joback Method

cpg	750.13	J/mol×K	893.00	Joback Method
cpg	762.08	J/mol×K	927.80	Joback Method
cpg	773.08	J/mol×K	962.60	Joback Method
cpg	783.16	J/mol×K	997.40	Joback Method

Sources

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=C22711531&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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