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

Inchi: InChI=1S/C19H26O4/c1-14(2)8-7-12-22-18(20)16-9-5-6-10-17(16)19(21)23-13-11-15(3)4

InchiKey: ODRADBFARMYZRD-UHFFFAOYSA-N

Formula: C19H26O4

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

Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	-179.11	kJ/mol	Joback Method
hf	-589.67	kJ/mol	Joback Method
hfus	38.08	kJ/mol	Joback Method
hvap	78.16	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.403		Crippen Method
mcvol	265.390	ml/mol	McGowan Method
pc	1503.48	kPa	Joback Method
rinpol	2198.00		NIST Webbook
tb	814.48	K	Joback Method
tc	1020.01	K	Joback Method
tf	456.43	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.49	J/mol×K	814.48	Joback Method
cpg	808.21	J/mol×K	848.74	Joback Method
cpg	822.84	J/mol×K	882.99	Joback Method
cpg	836.38	J/mol×K	917.25	Joback Method
cpg	848.86	J/mol×K	951.50	Joback Method
cpg	860.32	J/mol×K	985.76	Joback Method
cpg	870.77	J/mol×K	1020.01	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=U357103&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