Isophthalic acid, isohexyl 2-methylprop-2-en-1-yl ester

Inchi: InChI=1S/C18H24O4/c1-13(2)7-6-10-21-17(19)15-8-5-9-16(11-15)18(20)22-12-14(3)4/h5

InchiKey: ZTJXRPJDSMTFSF-UHFFFAOYSA-N

Formula: C18H24O4

SMILES: C=C(C)COC(=O)c1cccc(C(=O)OCCCC(C)C)c1

Mol. weight [g/mol]: 304.38

Physical Properties

Property code	Value	Unit	Source
gf	-187.53	kJ/mol	Joback Method
hf	-569.03	kJ/mol	Joback Method
hfus	35.49	kJ/mol	Joback Method
hvap	75.93	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.013		Crippen Method
mcvol	251.300	ml/mol	McGowan Method
pc	1621.98	kPa	Joback Method
rinpol	2239.00		NIST Webbook
rinpol	2239.00		NIST Webbook
tb	791.60	K	Joback Method
tc	998.20	K	Joback Method
tf	445.16	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.24	J/mol×K	791.60	Joback Method
cpg	750.76	J/mol×K	826.03	Joback Method
cpg	765.21	J/mol×K	860.47	Joback Method
cpg	778.60	J/mol×K	894.90	Joback Method
cpg	790.96	J/mol×K	929.33	Joback Method
cpg	802.31	J/mol×K	963.77	Joback Method
cpg	812.68	J/mol×K	998.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343948&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