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

Inchi: InChI=1S/C18H24O4/c1-4-5-6-7-11-21-17(19)15-9-8-10-16(12-15)18(20)22-13-14(2)3/h8

InchiKey: DBSHCMPAFZHMIF-UHFFFAOYSA-N

Formula: C18H24O4

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

Mol. weight [g/mol]: 304.38

Physical Properties

Property code	Value	Unit	Source
gf	-185.09	kJ/mol	Joback Method
hf	-563.75	kJ/mol	Joback Method
hfus	39.01	kJ/mol	Joback Method
hvap	76.32	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.157		Crippen Method
mcvol	251.300	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	2291.00		NIST Webbook
rinpol	2291.00		NIST Webbook
tb	792.04	K	Joback Method
tc	995.99	K	Joback Method
tf	460.16	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.70	J/mol×K	792.04	Joback Method
cpg	750.02	J/mol×K	826.03	Joback Method
cpg	764.30	J/mol×K	860.02	Joback Method
cpg	777.57	J/mol×K	894.02	Joback Method
cpg	789.84	J/mol×K	928.01	Joback Method
cpg	801.15	J/mol×K	962.00	Joback Method
cpg	811.50	J/mol×K	995.99	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=U343949&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