Isophthalic acid, isohexyl 3-methylbut-2-en-1-yl ester

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

InchiKey: SDNDULSPKLCURE-UHFFFAOYSA-N

Formula: C19H26O4

SMILES: CC(C)=CCOC(=O)c1cccc(C(=O)OCCCC(C)C)c1

Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	-186.73	kJ/mol	Joback Method
hf	-597.88	kJ/mol	Joback Method
hfus	39.56	kJ/mol	Joback Method
hvap	78.79	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.403		Crippen Method
mcvol	265.390	ml/mol	McGowan Method
pc	1515.21	kPa	Joback Method
rinpol	2399.00		NIST Webbook
tb	821.96	K	Joback Method
tc	1030.51	K	Joback Method
tf	453.11	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.23	J/mol×K	821.96	Joback Method
cpg	808.98	J/mol×K	856.72	Joback Method
cpg	823.63	J/mol×K	891.48	Joback Method
cpg	837.22	J/mol×K	926.24	Joback Method
cpg	849.79	J/mol×K	960.99	Joback Method
cpg	861.37	J/mol×K	995.75	Joback Method
cpg	871.98	J/mol×K	1030.51	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343937&Units=SI

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