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

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

InchiKey: YNNIZWILVAJUEW-UHFFFAOYSA-N

Formula: C19H26O4

SMILES: CCCCCCOC(=O)c1cccc(C(=O)OCC=C(C)C)c1

Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	-184.29	kJ/mol	Joback Method
hf	-592.60	kJ/mol	Joback Method
hfus	43.08	kJ/mol	Joback Method
hvap	79.18	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.547		Crippen Method
mcvol	265.390	ml/mol	McGowan Method
pc	1505.81	kPa	Joback Method
rinpol	2448.00		NIST Webbook
rinpol	2448.00		NIST Webbook
tb	822.40	K	Joback Method
tc	1028.52	K	Joback Method
tf	468.11	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.70	J/mol×K	822.40	Joback Method
cpg	808.27	J/mol×K	856.75	Joback Method
cpg	822.78	J/mol×K	891.11	Joback Method
cpg	836.27	J/mol×K	925.46	Joback Method
cpg	848.77	J/mol×K	959.82	Joback Method
cpg	860.31	J/mol×K	994.17	Joback Method
cpg	870.92	J/mol×K	1028.52	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=U343938&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