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

Inchi: InChI=1S/C18H24O4/c1-4-5-6-11-21-17(19)15-8-7-9-16(13-15)18(20)22-12-10-14(2)3/h7

InchiKey: UVROMVJOMZBTOP-UHFFFAOYSA-N

Formula: C18H24O4

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

Mol. weight [g/mol]: 304.38

Physical Properties

Property code	Value	Unit	Source
gf	-192.71	kJ/mol	Joback Method
hf	-571.96	kJ/mol	Joback Method
hfus	40.49	kJ/mol	Joback Method
hvap	76.95	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.157		Crippen Method
mcvol	251.300	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
rinpol	2343.00		NIST Webbook
rinpol	2343.00		NIST Webbook
tb	799.52	K	Joback Method
tc	1006.60	K	Joback Method
tf	456.84	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.37	J/mol×K	799.52	Joback Method
cpg	750.70	J/mol×K	834.03	Joback Method
cpg	765.01	J/mol×K	868.55	Joback Method
cpg	778.31	J/mol×K	903.06	Joback Method
cpg	790.64	J/mol×K	937.57	Joback Method
cpg	802.04	J/mol×K	972.09	Joback Method
cpg	812.52	J/mol×K	1006.60	Joback Method

Sources

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=U343936&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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