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

Inchi: InChI=1S/C15H18O4/c1-4-18-14(16)12-6-5-7-13(10-12)15(17)19-9-8-11(2)3/h5-8,10H,4,
InchiKey: ZYVGHCXQTKRSDG-UHFFFAOYSA-N
Formula: C15H18O4
SMILES: CCOC(=O)c1cccc(C(=O)OCC=C(C)C)c1
Mol. weight [g/mol]: 262.30

Physical Properties

Property code	Value	Unit	Source
gf	-217.97	kJ/mol	Joback Method
hf	-510.04	kJ/mol	Joback Method
hfus	32.72	kJ/mol	Joback Method
hvap	70.27	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	2.986		Crippen Method
mcvol	209.030	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinpol	2033.00		NIST Webbook
tb	730.88	K	Joback Method
tc	944.24	K	Joback Method
tf	423.03	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.35	J/mol×K	730.88	Joback Method
cpg	583.76	J/mol×K	766.44	Joback Method
cpg	597.22	J/mol×K	802.00	Joback Method
cpg	609.74	J/mol×K	837.56	Joback Method
cpg	621.37	J/mol×K	873.12	Joback Method
cpg	632.11	J/mol×K	908.68	Joback Method
cpg	641.99	J/mol×K	944.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343932&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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