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

Inchi: InChI=1S/C16H20O4/c1-11(2)9-19-15(17)13-6-5-7-14(8-13)16(18)20-10-12(3)4/h5-8,12H

InchiKey: LYYMINXRIAPCJW-UHFFFAOYSA-N

Formula: C16H20O4

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

Mol. weight [g/mol]: 276.33

Physical Properties

Property code	Value	Unit	Source
gf	-204.37	kJ/mol	Joback Method
hf	-527.75	kJ/mol	Joback Method
hfus	30.31	kJ/mol	Joback Method
hvap	71.48	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.232		Crippen Method
mcvol	223.120	ml/mol	McGowan Method
pc	1905.24	kPa	Joback Method
rinpol	2033.00		NIST Webbook
rinpol	2033.00		NIST Webbook
tb	745.84	K	Joback Method
tc	956.28	K	Joback Method
tf	422.62	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.67	J/mol×K	745.84	Joback Method
cpg	638.66	J/mol×K	780.91	Joback Method
cpg	652.64	J/mol×K	815.99	Joback Method
cpg	665.62	J/mol×K	851.06	Joback Method
cpg	677.61	J/mol×K	886.13	Joback Method
cpg	688.64	J/mol×K	921.20	Joback Method
cpg	698.73	J/mol×K	956.28	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=U343946&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