Isophthalic acid, but-3-yn-2-yl isobutyl ester

Inchi: InChI=1S/C16H18O4/c1-5-12(4)20-16(18)14-8-6-7-13(9-14)15(17)19-10-11(2)3/h1,6-9,1
InchiKey: CBSBBSDTGUIQRQ-UHFFFAOYSA-N
Formula: C16H18O4
SMILES: C#CC(C)OC(=O)c1cccc(C(=O)OCC(C)C)c1
Mol. weight [g/mol]: 274.31

Physical Properties

Property code	Value	Unit	Source
gf	-63.03	kJ/mol	Joback Method
hf	-356.77	kJ/mol	Joback Method
hfus	32.35	kJ/mol	Joback Method
hvap	71.54	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	2.678		Crippen Method
mcvol	218.820	ml/mol	McGowan Method
pc	2100.34	kPa	Joback Method
rinpol	1972.00		NIST Webbook
rinpol	1972.00		NIST Webbook
tb	738.96	K	Joback Method
tc	957.79	K	Joback Method
tf	470.31	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.92	J/mol×K	738.96	Joback Method
cpg	613.58	J/mol×K	775.43	Joback Method
cpg	627.20	J/mol×K	811.90	Joback Method
cpg	639.80	J/mol×K	848.38	Joback Method
cpg	651.39	J/mol×K	884.85	Joback Method
cpg	662.01	J/mol×K	921.32	Joback Method
cpg	671.66	J/mol×K	957.79	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=U343898&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