

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

Inchi:	InChI=1S/C16H18O4/c1-4-6-10-19-15(17)13-8-7-9-14(11-13)16(18)20-12(3)5-2/h2,7-9,1
InchiKey:	WVXZWILJUONDRS-UHFFFAOYSA-N
Formula:	C16H18O4
SMILES:	C#CC(C)OC(=O)c1cccc(C(=O)OCCCC)c1
Mol. weight [g/mol]:	274.31

Physical Properties

Property code	Value	Unit	Source
gf	-60.59	kJ/mol	Joback Method
hf	-351.49	kJ/mol	Joback Method
hfus	35.87	kJ/mol	Joback Method
hvap	71.93	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	2.822		Crippen Method
mcvol	218.820	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
rinpol	2022.00		NIST Webbook
rinpol	2022.00		NIST Webbook
tb	739.40	K	Joback Method
tc	954.59	K	Joback Method
tf	485.31	K	Joback Method
vc	0.828	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.35	J/mol×K	739.40	Joback Method
cpg	612.76	J/mol×K	775.26	Joback Method
cpg	626.17	J/mol×K	811.13	Joback Method
cpg	638.60	J/mol×K	846.99	Joback Method
cpg	650.08	J/mol×K	882.86	Joback Method
cpg	660.61	J/mol×K	918.72	Joback Method
cpg	670.23	J/mol×K	954.59	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U343899&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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