Isophthalic acid, di(but-3-yn-2-yl) ester

Inchi: InChI=1S/C16H14O4/c1-5-11(3)19-15(17)13-8-7-9-14(10-13)16(18)20-12(4)6-2/h1-2,7-1
InchiKey: VCYIIORTCZDJDT-UHFFFAOYSA-N
Formula: C16H14O4
SMILES: C#CC(C)OC(=O)c1cccc(C(=O)OC(C)C#C)c1
Mol. weight [g/mol]: 270.28

Physical Properties

Property code	Value	Unit	Source
gf	160.04	kJ/mol	Joback Method
hf	-64.87	kJ/mol	Joback Method
hfus	35.33	kJ/mol	Joback Method
hvap	71.40	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	2.044		Crippen Method
mcvol	210.220	ml/mol	McGowan Method
pc	2417.12	kPa	Joback Method
rinpol	1933.00		NIST Webbook
rinpol	1933.00		NIST Webbook
tb	729.08	K	Joback Method
tc	960.99	K	Joback Method
tf	517.28	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.36	J/mol×K	729.08	Joback Method
cpg	562.96	J/mol×K	767.73	Joback Method
cpg	575.54	J/mol×K	806.38	Joback Method
cpg	587.10	J/mol×K	845.03	Joback Method
cpg	597.69	J/mol×K	883.69	Joback Method
cpg	607.33	J/mol×K	922.34	Joback Method
cpg	616.06	J/mol×K	960.99	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343901&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
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