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

Inchi: InChI=1S/C15H16O4/c1-4-9-18-14(16)12-7-6-8-13(10-12)15(17)19-11(3)5-2/h2,6-8,10-1
InchiKey: YVXSZFPQXUADMW-UHFFFAOYSA-N
Formula: C15H16O4
SMILES: C#CC(C)OC(=O)c1cccc(C(=O)OCCC)c1
Mol. weight [g/mol]: 260.29

Physical Properties

Property code	Value	Unit	Source
gf	-69.01	kJ/mol	Joback Method
hf	-330.85	kJ/mol	Joback Method
hfus	33.28	kJ/mol	Joback Method
hvap	69.70	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	2.432		Crippen Method
mcvol	204.730	ml/mol	McGowan Method
pc	2280.59	kPa	Joback Method
rinpol	1918.00		NIST Webbook
tb	716.52	K	Joback Method
tc	934.85	K	Joback Method
tf	474.04	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.02	J/mol×K	716.52	Joback Method
cpg	559.04	J/mol×K	752.91	Joback Method
cpg	572.09	J/mol×K	789.30	Joback Method
cpg	584.19	J/mol×K	825.69	Joback Method
cpg	595.36	J/mol×K	862.08	Joback Method
cpg	605.61	J/mol×K	898.47	Joback Method
cpg	614.97	J/mol×K	934.85	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=U343897&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