Isophthalic acid, ethyl hex-4-yn-3-yl ester

Inchi: InChI=1S/C16H18O4/c1-4-8-14(5-2)20-16(18)13-10-7-9-12(11-13)15(17)19-6-3/h7,9-11,
InchiKey: YOGKTBSKCUCDEY-UHFFFAOYSA-N
Formula: C16H18O4
SMILES: CC#CC(CC)OC(=O)c1cccc(C(=O)OCC)c1
Mol. weight [g/mol]: 274.31

Physical Properties

Property code	Value	Unit	Source
gf	-80.86	kJ/mol	Joback Method
hf	-371.09	kJ/mol	Joback Method
hfus	36.02	kJ/mol	Joback Method
hvap	74.22	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	2.822		Crippen Method
mcvol	218.820	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	2088.00		NIST Webbook
rinpol	2088.00		NIST Webbook
tb	758.28	K	Joback Method
tc	981.87	K	Joback Method
tf	544.44	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.93	J/mol×K	758.28	Joback Method
cpg	615.69	J/mol×K	795.54	Joback Method
cpg	629.36	J/mol×K	832.81	Joback Method
cpg	641.97	J/mol×K	870.07	Joback Method
cpg	653.51	J/mol×K	907.34	Joback Method
cpg	664.00	J/mol×K	944.60	Joback Method
cpg	673.45	J/mol×K	981.87	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=U343837&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