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

Inchi: InChI=1S/C17H20O4/c1-4-8-15(6-3)21-17(19)14-10-7-9-13(12-14)16(18)20-11-5-2/h7,9-
InchiKey: FJWHHSIUKCPJQJ-UHFFFAOYSA-N
Formula: C17H20O4
SMILES: CC#CC(CC)OC(=O)c1cccc(C(=O)OCCC)c1
Mol. weight [g/mol]: 288.34

Physical Properties

Property code	Value	Unit	Source
gf	-72.44	kJ/mol	Joback Method
hf	-391.73	kJ/mol	Joback Method
hfus	38.61	kJ/mol	Joback Method
hvap	76.45	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	3.212		Crippen Method
mcvol	232.910	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	2183.00		NIST Webbook
rinpol	2183.00		NIST Webbook
tb	781.16	K	Joback Method
tc	1001.61	K	Joback Method
tf	555.71	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.90	J/mol×K	781.16	Joback Method
cpg	670.93	J/mol×K	817.90	Joback Method
cpg	684.86	J/mol×K	854.64	Joback Method
cpg	697.68	J/mol×K	891.39	Joback Method
cpg	709.41	J/mol×K	928.13	Joback Method
cpg	720.07	J/mol×K	964.87	Joback Method
cpg	729.66	J/mol×K	1001.61	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=U343838&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