Isophthalic acid, di(hex-4-yn-3-yl) ester

Inchi: InChI=1S/C20H22O4/c1-5-10-17(7-3)23-19(21)15-12-9-13-16(14-15)20(22)24-18(8-4)11
InchiKey: IQNSRDAIBRBRDG-UHFFFAOYSA-N
Formula: C20H22O4
SMILES: CC#CC(CC)OC(=O)c1cccc(C(=O)OC(C#CC)CC)c1
Mol. weight [g/mol]: 326.39

Physical Properties

Property code	Value	Unit	Source
gf	153.18	kJ/mol	Joback Method
hf	-186.63	kJ/mol	Joback Method
hfus	45.98	kJ/mol	Joback Method
hvap	84.89	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	3.604		Crippen Method
mcvol	266.580	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	2454.00		NIST Webbook
rinpol	2454.00		NIST Webbook
tb	858.36	K	Joback Method
tc	1092.54	K	Joback Method
tf	680.62	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.74	J/mol×K	858.36	Joback Method
cpg	789.90	J/mol×K	897.39	Joback Method
cpg	803.73	J/mol×K	936.42	Joback Method
cpg	816.25	J/mol×K	975.45	Joback Method
cpg	827.46	J/mol×K	1014.48	Joback Method
cpg	837.41	J/mol×K	1053.51	Joback Method
cpg	846.10	J/mol×K	1092.54	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=U343843&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