Isophthalic acid, di(2,7-dimethyloct-7-en-5-yn-4-yl) ester

Inchi: InChI=1S/C28H34O4/c1-19(2)12-14-25(16-21(5)6)31-27(29)23-10-9-11-24(18-23)28(30)
InchiKey: BNNGIDHFWUWUOI-UHFFFAOYSA-N
Formula: C28H34O4
SMILES: C=C(C)C#CC(CC(C)C)OC(=O)c1cccc(C(=O)OC(C#CC(=C)C)CC(C)C)c1
Mol. weight [g/mol]: 434.57

Physical Properties

Property code	Value	Unit	Source
gf	374.24	kJ/mol	Joback Method
hf	-131.03	kJ/mol	Joback Method
hfus	54.47	kJ/mol	Joback Method
hvap	100.74	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	5.989		Crippen Method
mcvol	370.700	ml/mol	McGowan Method
pc	1073.57	kPa	Joback Method
rinpol	2855.00		NIST Webbook
rinpol	2855.00		NIST Webbook
tb	1033.64	K	Joback Method
tc	1272.99	K	Joback Method
tf	709.34	K	Joback Method
vc	1.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1193.53	J/mol×K	1033.64	Joback Method
cpg	1208.50	J/mol×K	1073.53	Joback Method
cpg	1221.95	J/mol×K	1113.42	Joback Method
cpg	1233.97	J/mol×K	1153.32	Joback Method
cpg	1244.63	J/mol×K	1193.21	Joback Method
cpg	1254.00	J/mol×K	1233.10	Joback Method
cpg	1262.15	J/mol×K	1272.99	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=U343852&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