Isophthalic acid, 2,6-dimethylnon-1-en-3-yn-5-yl pentyl ester

Inchi: InChI=1S/C24H32O4/c1-6-8-9-16-27-23(25)20-12-10-13-21(17-20)24(26)28-22(15-14-18

InchiKey: IWBWKQOPLDEECG-UHFFFAOYSA-N

Formula: C24H32O4

SMILES: C=C(C)C#CC(OC(=O)c1cccc(C(=O)OCCCCC)c1)C(C)CCC

Mol. weight [g/mol]: 384.51

Physical Properties

Property code	Value	Unit	Source
gf	63.35	kJ/mol	Joback Method
hf	-425.85	kJ/mol	Joback Method
hfus	50.63	kJ/mol	Joback Method
hvap	91.05	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	5.575		Crippen Method
mcvol	327.240	ml/mol	McGowan Method
pc	1196.48	kPa	Joback Method
rinpol	2683.00		NIST Webbook
tb	937.44	K	Joback Method
tc	1157.19	K	Joback Method
tf	603.88	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1036.02	J/mol×K	937.44	Joback Method
cpg	1051.80	J/mol×K	974.07	Joback Method
cpg	1066.23	J/mol×K	1010.69	Joback Method
cpg	1079.35	J/mol×K	1047.32	Joback Method
cpg	1091.21	J/mol×K	1083.94	Joback Method
cpg	1101.84	J/mol×K	1120.57	Joback Method
cpg	1111.29	J/mol×K	1157.19	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=U343856&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