Isophthalic acid, 2,7-dimethyloct-7-en-5-yn-4-yl isobutyl ester

Inchi: InChI=1S/C22H28O4/c1-15(2)10-11-20(12-16(3)4)26-22(24)19-9-7-8-18(13-19)21(23)25

InchiKey: ASFNMFRQQWDLKI-UHFFFAOYSA-N

Formula: C22H28O4

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

Mol. weight [g/mol]: 356.46

Physical Properties

Property code	Value	Unit	Source
gf	44.07	kJ/mol	Joback Method
hf	-389.85	kJ/mol	Joback Method
hfus	41.92	kJ/mol	Joback Method
hvap	86.21	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	4.650		Crippen Method
mcvol	299.060	ml/mol	McGowan Method
pc	1380.93	kPa	Joback Method
rinpol	2460.00		NIST Webbook
tb	891.24	K	Joback Method
tc	1113.11	K	Joback Method
tf	566.34	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.87	J/mol×K	891.24	Joback Method
cpg	932.64	J/mol×K	928.22	Joback Method
cpg	947.09	J/mol×K	965.20	Joback Method
cpg	960.25	J/mol×K	1002.17	Joback Method
cpg	972.15	J/mol×K	1039.15	Joback Method
cpg	982.83	J/mol×K	1076.13	Joback Method
cpg	992.33	J/mol×K	1113.11	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=U343846&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