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

Inchi: InChI=1S/C22H28O4/c1-6-9-17(5)20(13-12-16(3)4)26-22(24)19-11-8-10-18(15-19)21(23

InchiKey: SMWWKDTVJDRBJN-UHFFFAOYSA-N

Formula: C22H28O4

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

Mol. weight [g/mol]: 356.46

Physical Properties

Property code	Value	Unit	Source
gf	46.51	kJ/mol	Joback Method
hf	-384.57	kJ/mol	Joback Method
hfus	45.45	kJ/mol	Joback Method
hvap	86.60	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	4.795		Crippen Method
mcvol	299.060	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2482.00		NIST Webbook
rinpol	2482.00		NIST Webbook
tb	891.68	K	Joback Method
tc	1111.16	K	Joback Method
tf	581.34	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.37	J/mol×K	891.68	Joback Method
cpg	932.01	J/mol×K	928.26	Joback Method
cpg	946.36	J/mol×K	964.84	Joback Method
cpg	959.46	J/mol×K	1001.42	Joback Method
cpg	971.34	J/mol×K	1038.00	Joback Method
cpg	982.05	J/mol×K	1074.58	Joback Method
cpg	991.60	J/mol×K	1111.16	Joback Method

Sources

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=U343854&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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