Isophthalic acid, 2-methyloct-5-yn-4-yl propyl ester

Inchi: InChI=1S/C20H26O4/c1-5-7-11-18(13-15(3)4)24-20(22)17-10-8-9-16(14-17)19(21)23-12

InchiKey: XEZITXFIYUGBEP-UHFFFAOYSA-N

Formula: C20H26O4

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

Mol. weight [g/mol]: 330.42

Physical Properties

Property code	Value	Unit	Source
gf	-49.62	kJ/mol	Joback Method
hf	-458.93	kJ/mol	Joback Method
hfus	42.86	kJ/mol	Joback Method
hvap	82.74	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	4.238		Crippen Method
mcvol	275.180	ml/mol	McGowan Method
pc	1533.06	kPa	Joback Method
rinpol	2367.00		NIST Webbook
rinpol	2367.00		NIST Webbook
tb	849.36	K	Joback Method
tc	1066.44	K	Joback Method
tf	574.52	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.13	J/mol×K	849.36	Joback Method
cpg	842.88	J/mol×K	885.54	Joback Method
cpg	857.38	J/mol×K	921.72	Joback Method
cpg	870.65	J/mol×K	957.90	Joback Method
cpg	882.71	J/mol×K	994.08	Joback Method
cpg	893.60	J/mol×K	1030.26	Joback Method
cpg	903.32	J/mol×K	1066.44	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=U343923&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