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

Inchi: InChI=1S/C21H28O4/c1-6-7-11-19(12-15(2)3)25-21(23)18-10-8-9-17(13-18)20(22)24-14

InchiKey: VLKXVQOGIQYDEF-UHFFFAOYSA-N

Formula: C21H28O4

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

Mol. weight [g/mol]: 344.44

Physical Properties

Property code	Value	Unit	Source
gf	-43.64	kJ/mol	Joback Method
hf	-484.85	kJ/mol	Joback Method
hfus	41.92	kJ/mol	Joback Method
hvap	84.58	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	4.484		Crippen Method
mcvol	289.270	ml/mol	McGowan Method
pc	1432.63	kPa	Joback Method
rinpol	2414.00		NIST Webbook
rinpol	2414.00		NIST Webbook
tb	871.80	K	Joback Method
tc	1090.27	K	Joback Method
tf	570.79	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.21	J/mol×K	871.80	Joback Method
cpg	902.20	J/mol×K	908.21	Joback Method
cpg	916.87	J/mol×K	944.62	Joback Method
cpg	930.24	J/mol×K	981.03	Joback Method
cpg	942.35	J/mol×K	1017.45	Joback Method
cpg	953.21	J/mol×K	1053.86	Joback Method
cpg	962.85	J/mol×K	1090.27	Joback Method

Sources

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=U343924&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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