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

Inchi: InChI=1S/C24H34O4/c1-5-7-9-10-11-16-27-23(25)20-13-12-14-21(18-20)24(26)28-22(15

InchiKey: JOFLMLHHBKQDIB-UHFFFAOYSA-N

Formula: C24H34O4

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

Mol. weight [g/mol]: 386.52

Physical Properties

Property code	Value	Unit	Source
gf	-15.94	kJ/mol	Joback Method
hf	-541.49	kJ/mol	Joback Method
hfus	53.22	kJ/mol	Joback Method
hvap	91.64	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	5.799		Crippen Method
mcvol	331.540	ml/mol	McGowan Method
pc	1158.50	kPa	Joback Method
rinpol	2758.00		NIST Webbook
rinpol	2758.00		NIST Webbook
tb	940.88	K	Joback Method
tc	1158.29	K	Joback Method
tf	619.60	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1065.47	J/mol×K	940.88	Joback Method
cpg	1081.52	J/mol×K	977.11	Joback Method
cpg	1096.18	J/mol×K	1013.35	Joback Method
cpg	1109.46	J/mol×K	1049.58	Joback Method
cpg	1121.42	J/mol×K	1085.82	Joback Method
cpg	1132.09	J/mol×K	1122.05	Joback Method
cpg	1141.49	J/mol×K	1158.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343929&Units=SI
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

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