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

Inchi: InChI=1S/C23H32O4/c1-5-7-9-10-15-26-22(24)19-12-11-13-20(17-19)23(25)27-21(14-8-

InchiKey: UKAURQDLOZPEKG-UHFFFAOYSA-N

Formula: C23H32O4

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

Mol. weight [g/mol]: 372.50

Physical Properties

Property code	Value	Unit	Source
gf	-24.36	kJ/mol	Joback Method
hf	-520.85	kJ/mol	Joback Method
hfus	50.63	kJ/mol	Joback Method
hvap	89.42	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	5.409		Crippen Method
mcvol	317.450	ml/mol	McGowan Method
pc	1238.09	kPa	Joback Method
rinpol	2664.00		NIST Webbook
rinpol	2664.00		NIST Webbook
tb	918.00	K	Joback Method
tc	1134.16	K	Joback Method
tf	608.33	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.93	J/mol×K	918.00	Joback Method
cpg	1020.91	J/mol×K	954.03	Joback Method
cpg	1035.54	J/mol×K	990.05	Joback Method
cpg	1048.85	J/mol×K	1026.08	Joback Method
cpg	1060.86	J/mol×K	1062.11	Joback Method
cpg	1071.62	J/mol×K	1098.13	Joback Method
cpg	1081.15	J/mol×K	1134.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343928&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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