Isophthalic acid, hex-4-yn-3-yl hexyl ester

Inchi: InChI=1S/C20H26O4/c1-4-7-8-9-14-23-19(21)16-12-10-13-17(15-16)20(22)24-18(6-3)11
InchiKey: XBFDISZTYYNSMM-UHFFFAOYSA-N
Formula: C20H26O4
SMILES: CC#CC(CC)OC(=O)c1cccc(C(=O)OCCCCCC)c1
Mol. weight [g/mol]: 330.42

Physical Properties

Property code	Value	Unit	Source
gf	-47.18	kJ/mol	Joback Method
hf	-453.65	kJ/mol	Joback Method
hfus	46.38	kJ/mol	Joback Method
hvap	83.13	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	4.382		Crippen Method
mcvol	275.180	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	2496.00		NIST Webbook
rinpol	2496.00		NIST Webbook
tb	849.80	K	Joback Method
tc	1064.28	K	Joback Method
tf	589.52	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.60	J/mol×K	849.80	Joback Method
cpg	842.18	J/mol×K	885.55	Joback Method
cpg	856.55	J/mol×K	921.29	Joback Method
cpg	869.73	J/mol×K	957.04	Joback Method
cpg	881.75	J/mol×K	992.79	Joback Method
cpg	892.63	J/mol×K	1028.53	Joback Method
cpg	902.38	J/mol×K	1064.28	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=U343842&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