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

Inchi: InChI=1S/C18H22O4/c1-5-8-16(6-2)22-18(20)15-10-7-9-14(11-15)17(19)21-12-13(3)4/h7
InchiKey: MTVZROXWOUNCBB-UHFFFAOYSA-N
Formula: C18H22O4
SMILES: CC#CC(CC)OC(=O)c1cccc(C(=O)OCC(C)C)c1
Mol. weight [g/mol]: 302.36

Physical Properties

Property code	Value	Unit	Source
gf	-66.46	kJ/mol	Joback Method
hf	-417.65	kJ/mol	Joback Method
hfus	37.68	kJ/mol	Joback Method
hvap	78.29	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.458		Crippen Method
mcvol	247.000	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	2235.00		NIST Webbook
rinpol	2235.00		NIST Webbook
tb	803.60	K	Joback Method
tc	1024.70	K	Joback Method
tf	551.98	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.44	J/mol×K	803.60	Joback Method
cpg	727.92	J/mol×K	840.45	Joback Method
cpg	742.20	J/mol×K	877.30	Joback Method
cpg	755.31	J/mol×K	914.15	Joback Method
cpg	767.27	J/mol×K	951.00	Joback Method
cpg	778.08	J/mol×K	987.85	Joback Method
cpg	787.76	J/mol×K	1024.70	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=U343839&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