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

Inchi: InChI=1S/C23H32O4/c1-6-7-13-21(15-18(4)5)27-23(25)20-12-8-11-19(16-20)22(24)26-1
InchiKey: JWYWZFZLXFGIHQ-UHFFFAOYSA-N
Formula: C23H32O4
SMILES: CCC#CC(CC(C)C)OC(=O)c1cccc(C(=O)OCCCC(C)C)c1
Mol. weight [g/mol]: 372.50

Physical Properties

Property code	Value	Unit	Source
gf	-26.80	kJ/mol	Joback Method
hf	-526.13	kJ/mol	Joback Method
hfus	47.10	kJ/mol	Joback Method
hvap	89.03	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.264		Crippen Method
mcvol	317.450	ml/mol	McGowan Method
pc	1245.09	kPa	Joback Method
rinpol	2616.00		NIST Webbook
rinpol	2616.00		NIST Webbook
tb	917.56	K	Joback Method
tc	1135.45	K	Joback Method
tf	593.33	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1005.40	J/mol×K	917.56	Joback Method
cpg	1021.47	J/mol×K	953.88	Joback Method
cpg	1036.15	J/mol×K	990.19	Joback Method
cpg	1049.48	J/mol×K	1026.51	Joback Method
cpg	1061.48	J/mol×K	1062.82	Joback Method
cpg	1072.20	J/mol×K	1099.14	Joback Method
cpg	1081.65	J/mol×K	1135.45	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=U343927&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