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

Inchi: InChI=1S/C22H30O4/c1-5-7-9-14-25-21(23)18-11-10-12-19(16-18)22(24)26-20(13-8-6-2
InchiKey: OKWYTSNPMYGYRL-UHFFFAOYSA-N
Formula: C22H30O4
SMILES: CCC#CC(CC(C)C)OC(=O)c1cccc(C(=O)OCCCCC)c1
Mol. weight [g/mol]: 358.47

Physical Properties

Property code	Value	Unit	Source
gf	-32.78	kJ/mol	Joback Method
hf	-500.21	kJ/mol	Joback Method
hfus	48.04	kJ/mol	Joback Method
hvap	87.19	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	5.018		Crippen Method
mcvol	303.360	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
rinpol	2564.00		NIST Webbook
tb	895.12	K	Joback Method
tc	1110.84	K	Joback Method
tf	597.06	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.99	J/mol×K	895.12	Joback Method
cpg	960.90	J/mol×K	931.07	Joback Method
cpg	975.50	J/mol×K	967.03	Joback Method
cpg	988.81	J/mol×K	1002.98	Joback Method
cpg	1000.87	J/mol×K	1038.94	Joback Method
cpg	1011.69	J/mol×K	1074.89	Joback Method
cpg	1021.31	J/mol×K	1110.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343926&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