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

Inchi: InChI=1S/C25H36O4/c1-5-7-9-10-11-12-17-28-24(26)21-14-13-15-22(19-21)25(27)29-23

InchiKey: RYSNLKMTXDTVRL-UHFFFAOYSA-N

Formula: C25H36O4

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

Mol. weight [g/mol]: 400.55

Physical Properties

Property code	Value	Unit	Source
gf	-7.52	kJ/mol	Joback Method
hf	-562.13	kJ/mol	Joback Method
hfus	55.81	kJ/mol	Joback Method
hvap	93.87	kJ/mol	Joback Method
log10ws	-7.90		Crippen Method
logp	6.189		Crippen Method
mcvol	345.630	ml/mol	McGowan Method
pc	1086.35	kPa	Joback Method
rinpol	2857.00		NIST Webbook
rinpol	2857.00		NIST Webbook
tb	963.76	K	Joback Method
tc	1183.28	K	Joback Method
tf	630.87	K	Joback Method
vc	1.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.54	J/mol×K	963.76	Joback Method
cpg	1142.67	J/mol×K	1000.35	Joback Method
cpg	1157.35	J/mol×K	1036.93	Joback Method
cpg	1170.61	J/mol×K	1073.52	Joback Method
cpg	1182.50	J/mol×K	1110.11	Joback Method
cpg	1193.06	J/mol×K	1146.69	Joback Method
cpg	1202.32	J/mol×K	1183.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343930&Units=SI

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