Isophthalic acid, 2,7-dimethyloct-7-en-5-yn-4-yl heptyl ester

Inchi: InChI=1S/C25H34O4/c1-6-7-8-9-10-16-28-24(26)21-12-11-13-22(18-21)25(27)29-23(17-

InchiKey: MNDXCRVBAXCLDX-UHFFFAOYSA-N

Formula: C25H34O4

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

Mol. weight [g/mol]: 398.54

Physical Properties

Property code	Value	Unit	Source
gf	71.77	kJ/mol	Joback Method
hf	-446.49	kJ/mol	Joback Method
hfus	53.22	kJ/mol	Joback Method
hvap	93.28	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	5.965		Crippen Method
mcvol	341.330	ml/mol	McGowan Method
pc	1120.80	kPa	Joback Method
rinpol	2799.00		NIST Webbook
rinpol	2799.00		NIST Webbook
tb	960.32	K	Joback Method
tc	1181.44	K	Joback Method
tf	615.15	K	Joback Method
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1096.73	J/mol×K	960.32	Joback Method
cpg	1112.59	J/mol×K	997.17	Joback Method
cpg	1127.06	J/mol×K	1034.03	Joback Method
cpg	1140.18	J/mol×K	1070.88	Joback Method
cpg	1152.00	J/mol×K	1107.73	Joback Method
cpg	1162.57	J/mol×K	1144.59	Joback Method
cpg	1171.94	J/mol×K	1181.44	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=U343851&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