Bis(3,7-dimethyloct-6-enyl) phthalate

Other names: 1,2-Benzenedicarboxylic acid, bis(3,7-dimethyloct-6-enyl) ester
Bis(3,7-dimethyloct-6-enyl)-1,2-benzenedicarboxylate
Inchi: InChI=1S/C28H42O4/c1-21(2)11-9-13-23(5)17-19-31-27(29)25-15-7-8-16-26(25)28(30)3
InchiKey: ZHDJIKXYGTXDLO-UHFFFAOYSA-N
Formula: C28H42O4
SMILES: CC(C)=CCCC(C)CCOC(=O)c1ccccc1C(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 442.63

Physical Properties

Property code	Value	Unit	Source
gf	-41.72	kJ/mol	Joback Method
hf	-681.49	kJ/mol	Joback Method
hfus	58.24	kJ/mol	Joback Method
hvap	98.47	kJ/mol	Joback Method
log10ws	-8.72		Crippen Method
logp	7.545		Crippen Method
mcvol	387.900	ml/mol	McGowan Method
pc	881.57	kPa	Joback Method
rinpol	3081.00		NIST Webbook
tb	1031.48	K	Joback Method
tc	1262.88	K	Joback Method
tf	520.50	K	Joback Method
vc	1.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1312.16	J/mol×K	1031.48	Joback Method
cpg	1329.79	J/mol×K	1070.05	Joback Method
cpg	1346.10	J/mol×K	1108.61	Joback Method
cpg	1361.19	J/mol×K	1147.18	Joback Method
cpg	1375.16	J/mol×K	1185.75	Joback Method
cpg	1388.11	J/mol×K	1224.32	Joback Method
cpg	1400.13	J/mol×K	1262.88	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=U373645&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