Isophthalic acid, 3,7-dimethyloct-6-enyl pentyl ester

Inchi: InChI=1S/C23H34O4/c1-5-6-7-15-26-22(24)20-12-9-13-21(17-20)23(25)27-16-14-19(4)11-8-10-18(2)3/h9,12-13,17,19H,5-8,10-11,14-16H2,1-4H3/b18-10+

InchiKey: MTDRXODTLKKFRY-UHFFFAOYSA-N

Formula: C23H34O4

SMILES: CCCCCOC(=O)c1cccc(C(=O)OCCC(C)CCC=C(C)C)c1

Mol. weight [g/mol]: 374.51

Physical Properties

Property code	Value	Unit	Source
gf	-153.05	kJ/mol	Joback Method
hf	-680.44	kJ/mol	Joback Method
hfus	49.92	kJ/mol	Joback Method
hvap	87.69	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	5.963		Crippen Method
mcvol	321.750	ml/mol	McGowan Method
pc	1146.76	kPa	Joback Method
rinpol	2683.00		NIST Webbook
tb	913.48	K	Joback Method
tc	1123.80	K	Joback Method
tf	498.19	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.55	J/mol×K	913.48	Joback Method
cpg	1047.05	J/mol×K	948.53	Joback Method
cpg	1062.33	J/mol×K	983.59	Joback Method
cpg	1076.43	J/mol×K	1018.64	Joback Method
cpg	1089.41	J/mol×K	1053.69	Joback Method
cpg	1101.31	J/mol×K	1088.75	Joback Method
cpg	1112.17	J/mol×K	1123.80	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=U356739&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