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

Inchi: InChI=1S/C22H32O4/c1-5-6-14-25-21(23)19-11-8-12-20(16-19)22(24)26-15-13-18(4)10-

InchiKey: NNFZFKXSYYBMLW-UHFFFAOYSA-N

Formula: C22H32O4

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

Mol. weight [g/mol]: 360.49

Physical Properties

Property code	Value	Unit	Source
gf	-161.47	kJ/mol	Joback Method
hf	-659.80	kJ/mol	Joback Method
hfus	47.33	kJ/mol	Joback Method
hvap	85.47	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.573		Crippen Method
mcvol	307.660	ml/mol	McGowan Method
pc	1225.12	kPa	Joback Method
rinpol	2587.00		NIST Webbook
tb	890.60	K	Joback Method
tc	1099.35	K	Joback Method
tf	486.92	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.14	J/mol×K	890.60	Joback Method
cpg	986.45	J/mol×K	925.39	Joback Method
cpg	1001.58	J/mol×K	960.18	Joback Method
cpg	1015.56	J/mol×K	994.98	Joback Method
cpg	1028.45	J/mol×K	1029.77	Joback Method
cpg	1040.28	J/mol×K	1064.56	Joback Method
cpg	1051.10	J/mol×K	1099.35	Joback Method

Sources

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=U356738&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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