Isophthalic acid, 3-methylbut-2-en-1-yl nonyl ester

Inchi: InChI=1S/C22H32O4/c1-4-5-6-7-8-9-10-15-25-21(23)19-12-11-13-20(17-19)22(24)26-16
InchiKey: ZFXUQHXZQKWQMU-UHFFFAOYSA-N
Formula: C22H32O4
SMILES: CCCCCCCCCOC(=O)c1cccc(C(=O)OCC=C(C)C)c1
Mol. weight [g/mol]: 360.49

Physical Properties

Property code	Value	Unit	Source
gf	-159.03	kJ/mol	Joback Method
hf	-654.52	kJ/mol	Joback Method
hfus	50.85	kJ/mol	Joback Method
hvap	85.85	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	5.717		Crippen Method
mcvol	307.660	ml/mol	McGowan Method
pc	1218.29	kPa	Joback Method
rinpol	2754.00		NIST Webbook
rinpol	2754.00		NIST Webbook
tb	891.04	K	Joback Method
tc	1098.35	K	Joback Method
tf	501.92	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.66	J/mol×K	891.04	Joback Method
cpg	985.88	J/mol×K	925.59	Joback Method
cpg	1000.95	J/mol×K	960.14	Joback Method
cpg	1014.90	J/mol×K	994.69	Joback Method
cpg	1027.78	J/mol×K	1029.24	Joback Method
cpg	1039.64	J/mol×K	1063.80	Joback Method
cpg	1050.51	J/mol×K	1098.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343941&Units=SI
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

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