Phthalic acid, 3-methylbut-3-enyl nonyl ester

Inchi: InChI=1S/C22H32O4/c1-4-5-6-7-8-9-12-16-25-21(23)19-13-10-11-14-20(19)22(24)26-17
InchiKey: OZBIAARGFSXAPO-UHFFFAOYSA-N
Formula: C22H32O4
SMILES: C=C(C)CCOC(=O)c1ccccc1C(=O)OCCCCCCCCC
Mol. weight [g/mol]: 360.49

Physical Properties

Property code	Value	Unit	Source
gf	-151.41	kJ/mol	Joback Method
hf	-646.31	kJ/mol	Joback Method
hfus	49.37	kJ/mol	Joback Method
hvap	85.23	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	5.717		Crippen Method
mcvol	307.660	ml/mol	McGowan Method
pc	1209.83	kPa	Joback Method
rinpol	2535.00		NIST Webbook
rinpol	2535.00		NIST Webbook
tb	883.56	K	Joback Method
tc	1088.50	K	Joback Method
tf	505.24	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	968.67	J/mol×K	883.56	Joback Method
cpg	984.85	J/mol×K	917.72	Joback Method
cpg	999.85	J/mol×K	951.87	Joback Method
cpg	1013.69	J/mol×K	986.03	Joback Method
cpg	1026.40	J/mol×K	1020.19	Joback Method
cpg	1038.03	J/mol×K	1054.34	Joback Method
cpg	1048.60	J/mol×K	1088.50	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=U357107&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