Phthalic acid, 5-ethyl-1,3-dioxan-5-yl nonyl ester

Inchi: InChI=1S/C24H36O6/c1-3-5-6-7-8-9-12-15-29-22(25)20-13-10-11-14-21(20)23(26)30-18
InchiKey: LCTSBXULSPASMD-UHFFFAOYSA-N
Formula: C24H36O6
SMILES: CCCCCCCCCOC(=O)c1ccccc1C(=O)OCC1(CC)COCOC1
Mol. weight [g/mol]: 420.54

Physical Properties

Property code	Value	Unit	Source
gf	-367.14	kJ/mol	Joback Method
hf	-997.67	kJ/mol	Joback Method
hfus	58.64	kJ/mol	Joback Method
hvap	98.57	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	5.152		Crippen Method
mcvol	341.020	ml/mol	McGowan Method
pc	1203.96	kPa	Joback Method
rinpol	3194.00		NIST Webbook
rinpol	3194.00		NIST Webbook
tb	1006.45	K	Joback Method
tc	1234.66	K	Joback Method
tf	627.92	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1185.90	J/mol×K	1006.45	Joback Method
cpg	1205.93	J/mol×K	1044.48	Joback Method
cpg	1225.37	J/mol×K	1082.52	Joback Method
cpg	1244.38	J/mol×K	1120.55	Joback Method
cpg	1263.10	J/mol×K	1158.59	Joback Method
cpg	1281.67	J/mol×K	1196.62	Joback Method
cpg	1300.23	J/mol×K	1234.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415485&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