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

Inchi: InChI=1S/C26H40O6/c1-3-5-6-7-8-9-10-11-14-17-31-24(27)22-15-12-13-16-23(22)25(28

InchiKey: RHZWBSDIJYPVAE-UHFFFAOYSA-N

Formula: C26H40O6

SMILES: CCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCC1(CC)COCOC1

Mol. weight [g/mol]: 448.59

Physical Properties

Property code	Value	Unit	Source
gf	-350.30	kJ/mol	Joback Method
hf	-1038.95	kJ/mol	Joback Method
hfus	63.82	kJ/mol	Joback Method
hvap	103.02	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	5.932		Crippen Method
mcvol	369.200	ml/mol	McGowan Method
pc	1058.26	kPa	Joback Method
rinpol	3031.00		NIST Webbook
rinpol	3031.00		NIST Webbook
tb	1052.21	K	Joback Method
tc	1288.21	K	Joback Method
tf	650.46	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.29	J/mol×K	1052.21	Joback Method
cpg	1336.82	J/mol×K	1091.54	Joback Method
cpg	1357.82	J/mol×K	1130.88	Joback Method
cpg	1378.45	J/mol×K	1170.21	Joback Method
cpg	1398.90	J/mol×K	1209.54	Joback Method
cpg	1419.33	J/mol×K	1248.88	Joback Method
cpg	1439.90	J/mol×K	1288.21	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=U415487&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