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

Inchi: InChI=1S/C27H42O6/c1-3-5-6-7-8-9-10-11-12-15-18-32-25(28)23-16-13-14-17-24(23)26
InchiKey: CMOQWNPBWLNGRA-UHFFFAOYSA-N
Formula: C27H42O6
SMILES: CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCC1(CC)COCOC1
Mol. weight [g/mol]: 462.62

Physical Properties

Property code	Value	Unit	Source
gf	-341.88	kJ/mol	Joback Method
hf	-1059.59	kJ/mol	Joback Method
hfus	66.41	kJ/mol	Joback Method
hvap	105.24	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	6.322		Crippen Method
mcvol	383.290	ml/mol	McGowan Method
pc	995.13	kPa	Joback Method
rinpol	2105.00		NIST Webbook
tb	1075.09	K	Joback Method
tc	1316.63	K	Joback Method
tf	661.73	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1381.02	J/mol×K	1075.09	Joback Method
cpg	1403.46	J/mol×K	1115.35	Joback Method
cpg	1425.41	J/mol×K	1155.60	Joback Method
cpg	1447.05	J/mol×K	1195.86	Joback Method
cpg	1468.57	J/mol×K	1236.12	Joback Method
cpg	1490.16	J/mol×K	1276.38	Joback Method
cpg	1511.99	J/mol×K	1316.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415488&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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