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

Inchi: InChI=1S/C25H38O6/c1-3-5-6-7-8-9-10-13-16-30-23(26)21-14-11-12-15-22(21)24(27)31
InchiKey: BRGJTFZTNFHHCL-UHFFFAOYSA-N
Formula: C25H38O6
SMILES: CCCCCCCCCCOC(=O)c1ccccc1C(=O)OCC1(CC)COCOC1
Mol. weight [g/mol]: 434.57

Physical Properties

Property code	Value	Unit	Source
gf	-358.72	kJ/mol	Joback Method
hf	-1018.31	kJ/mol	Joback Method
hfus	61.23	kJ/mol	Joback Method
hvap	100.79	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	5.542		Crippen Method
mcvol	355.110	ml/mol	McGowan Method
pc	1127.59	kPa	Joback Method
rinpol	3297.00		NIST Webbook
tb	1029.33	K	Joback Method
tc	1260.91	K	Joback Method
tf	639.19	K	Joback Method
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1250.24	J/mol×K	1029.33	Joback Method
cpg	1270.97	J/mol×K	1067.93	Joback Method
cpg	1291.14	J/mol×K	1106.52	Joback Method
cpg	1310.91	J/mol×K	1145.12	Joback Method
cpg	1330.43	J/mol×K	1183.72	Joback Method
cpg	1349.86	J/mol×K	1222.31	Joback Method
cpg	1369.36	J/mol×K	1260.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415486&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