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

Inchi: InChI=1S/C23H34O6/c1-3-5-6-7-8-11-14-28-21(24)19-12-9-10-13-20(19)22(25)29-17-23

InchiKey: OSUNTTFZNDIIDA-UHFFFAOYSA-N

Formula: C23H34O6

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

Mol. weight [g/mol]: 406.51

Physical Properties

Property code	Value	Unit	Source
gf	-375.56	kJ/mol	Joback Method
hf	-977.03	kJ/mol	Joback Method
hfus	56.05	kJ/mol	Joback Method
hvap	96.34	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.761		Crippen Method
mcvol	326.930	ml/mol	McGowan Method
pc	1288.36	kPa	Joback Method
rinpol	3090.00		NIST Webbook
rinpol	3090.00		NIST Webbook
tb	983.57	K	Joback Method
tc	1209.39	K	Joback Method
tf	616.65	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1122.28	J/mol×K	983.57	Joback Method
cpg	1141.70	J/mol×K	1021.21	Joback Method
cpg	1160.51	J/mol×K	1058.84	Joback Method
cpg	1178.86	J/mol×K	1096.48	Joback Method
cpg	1196.86	J/mol×K	1134.12	Joback Method
cpg	1214.68	J/mol×K	1171.75	Joback Method
cpg	1232.43	J/mol×K	1209.39	Joback Method

Sources

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=U415484&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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