Isophthalic acid, 2-methylprop-2-en-1-yl undecyl ester

Inchi: InChI=1S/C23H34O4/c1-4-5-6-7-8-9-10-11-12-16-26-22(24)20-14-13-15-21(17-20)23(25
InchiKey: VDOVZIWCQHESRM-UHFFFAOYSA-N
Formula: C23H34O4
SMILES: C=C(C)COC(=O)c1cccc(C(=O)OCCCCCCCCCCC)c1
Mol. weight [g/mol]: 374.51

Physical Properties

Property code	Value	Unit	Source
gf	-142.99	kJ/mol	Joback Method
hf	-666.95	kJ/mol	Joback Method
hfus	51.96	kJ/mol	Joback Method
hvap	87.45	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	6.107		Crippen Method
mcvol	321.750	ml/mol	McGowan Method
pc	1132.91	kPa	Joback Method
rinpol	2806.00		NIST Webbook
rinpol	2806.00		NIST Webbook
tb	906.44	K	Joback Method
tc	1113.48	K	Joback Method
tf	516.51	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1029.01	J/mol×K	906.44	Joback Method
cpg	1045.41	J/mol×K	940.95	Joback Method
cpg	1060.56	J/mol×K	975.45	Joback Method
cpg	1074.52	J/mol×K	1009.96	Joback Method
cpg	1087.31	J/mol×K	1044.47	Joback Method
cpg	1098.97	J/mol×K	1078.97	Joback Method
cpg	1109.54	J/mol×K	1113.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343954&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

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