Isophthalic acid, butyl undec-2-en-1-yl ester

Inchi: InChI=1S/C23H34O4/c1-3-5-7-8-9-10-11-12-13-18-27-23(25)21-16-14-15-20(19-21)22(2
InchiKey: JTNIHRKQZCSKDM-OUKQBFOZSA-N
Formula: C23H34O4
SMILES: CCCCCCCCC=CCOC(=O)c1cccc(C(=O)OCCCC)c1
Mol. weight [g/mol]: 374.51

Physical Properties

Property code	Value	Unit	Source
gf	-142.06	kJ/mol	Joback Method
hf	-665.37	kJ/mol	Joback Method
hfus	54.75	kJ/mol	Joback Method
hvap	88.00	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	6.107		Crippen Method
mcvol	321.750	ml/mol	McGowan Method
pc	1136.73	kPa	Joback Method
rinpol	2846.00		NIST Webbook
rinpol	2846.00		NIST Webbook
tb	914.04	K	Joback Method
tc	1122.42	K	Joback Method
tf	527.15	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.46	J/mol×K	914.04	Joback Method
cpg	1046.83	J/mol×K	948.77	Joback Method
cpg	1062.01	J/mol×K	983.50	Joback Method
cpg	1076.03	J/mol×K	1018.23	Joback Method
cpg	1088.95	J/mol×K	1052.96	Joback Method
cpg	1100.82	J/mol×K	1087.69	Joback Method
cpg	1111.67	J/mol×K	1122.42	Joback Method
dvisc	0.0003985	Pa×s	527.15	Joback Method

dvisc	0.0002069	Pa×s	591.63	Joback Method
dvisc	0.0001222	Pa×s	656.11	Joback Method
dvisc	0.0000793	Pa×s	720.59	Joback Method
dvisc	0.0000552	Pa×s	785.08	Joback Method
dvisc	0.0000406	Pa×s	849.56	Joback Method
dvisc	0.0000312	Pa×s	914.04	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=U343905&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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