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

Inchi: InChI=1S/C21H30O4/c1-3-5-6-7-8-9-10-11-12-16-25-21(23)19-15-13-14-18(17-19)20(22
InchiKey: ZLRIRIASERYGJM-VAWYXSNFSA-N
Formula: C21H30O4
SMILES: CCCCCCCCC=CCOC(=O)c1cccc(C(=O)OCC)c1
Mol. weight [g/mol]: 346.46

Physical Properties

Property code	Value	Unit	Source
gf	-158.90	kJ/mol	Joback Method
hf	-624.09	kJ/mol	Joback Method
hfus	49.57	kJ/mol	Joback Method
hvap	83.55	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.327		Crippen Method
mcvol	293.570	ml/mol	McGowan Method
pc	1299.53	kPa	Joback Method
rinpol	2653.00		NIST Webbook
rinpol	2653.00		NIST Webbook
tb	868.28	K	Joback Method
tc	1073.05	K	Joback Method
tf	504.61	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.28	J/mol×K	868.28	Joback Method
cpg	926.18	J/mol×K	902.41	Joback Method
cpg	940.96	J/mol×K	936.54	Joback Method
cpg	954.67	J/mol×K	970.67	Joback Method
cpg	967.35	J/mol×K	1004.80	Joback Method
cpg	979.03	J/mol×K	1038.92	Joback Method
cpg	989.75	J/mol×K	1073.05	Joback Method
dvisc	0.0004944	Pa×s	504.61	Joback Method

dvisc	0.0002623	Pa×s	565.22	Joback Method
dvisc	0.0001573	Pa×s	625.83	Joback Method
dvisc	0.0001033	Pa×s	686.44	Joback Method
dvisc	0.0000726	Pa×s	747.06	Joback Method
dvisc	0.0000538	Pa×s	807.67	Joback Method
dvisc	0.0000416	Pa×s	868.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343902&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
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