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

Inchi: InChI=1S/C22H32O4/c1-3-5-6-7-8-9-10-11-12-17-26-22(24)20-15-13-14-19(18-20)21(23
InchiKey: FKGQQZRBLJIGPW-VAWYXSNFSA-N
Formula: C22H32O4
SMILES: CCCCCCCCC=CCOC(=O)c1cccc(C(=O)OCCC)c1
Mol. weight [g/mol]: 360.49

Physical Properties

Property code	Value	Unit	Source
gf	-150.48	kJ/mol	Joback Method
hf	-644.73	kJ/mol	Joback Method
hfus	52.16	kJ/mol	Joback Method
hvap	85.77	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	5.717		Crippen Method
mcvol	307.660	ml/mol	McGowan Method
pc	1214.05	kPa	Joback Method
rinpol	2747.00		NIST Webbook
rinpol	2747.00		NIST Webbook
tb	891.16	K	Joback Method
tc	1097.33	K	Joback Method
tf	515.88	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.03	J/mol×K	891.16	Joback Method
cpg	986.16	J/mol×K	925.52	Joback Method
cpg	1001.14	J/mol×K	959.88	Joback Method
cpg	1015.00	J/mol×K	994.25	Joback Method
cpg	1027.80	J/mol×K	1028.61	Joback Method
cpg	1039.58	J/mol×K	1062.97	Joback Method
cpg	1050.37	J/mol×K	1097.33	Joback Method
dvisc	0.0004447	Pa×s	515.88	Joback Method

dvisc	0.0002333	Pa×s	578.43	Joback Method
dvisc	0.0001388	Pa×s	640.97	Joback Method
dvisc	0.0000906	Pa×s	703.52	Joback Method
dvisc	0.0000634	Pa×s	766.07	Joback Method
dvisc	0.0000468	Pa×s	828.61	Joback Method
dvisc	0.0000361	Pa×s	891.16	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=U343903&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