Phthalic acid, propyl trans-dec-3-enyl ester

Inchi: InChI=1S/C21H30O4/c1-3-5-6-7-8-9-10-13-17-25-21(23)19-15-12-11-14-18(19)20(22)24
InchiKey: KFPLEVXTZBRRSU-MDZDMXLPSA-N
Formula: C21H30O4
SMILES: CCCCCCC=CCCOC(=O)c1ccccc1C(=O)OCCC
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	2454.00		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	979.03	J/mol×K	1038.92	Joback Method
cpg	967.35	J/mol×K	1004.80	Joback Method
cpg	954.67	J/mol×K	970.67	Joback Method
cpg	940.96	J/mol×K	936.54	Joback Method
cpg	926.18	J/mol×K	902.41	Joback Method
cpg	989.75	J/mol×K	1073.05	Joback Method
dvisc	0.0000416	Pa×s	868.28	Joback Method
dvisc	0.0000538	Pa×s	807.67	Joback Method

dvisc	0.0000726	Pa×s	747.06	Joback Method
dvisc	0.0001033	Pa×s	686.44	Joback Method
dvisc	0.0001573	Pa×s	625.83	Joback Method
dvisc	0.0002623	Pa×s	565.22	Joback Method
dvisc	0.0004944	Pa×s	504.61	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U360498&Units=SI

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