Isophthalic acid, octyl pent-4-enyl ester

Inchi: InChI=1S/C21H30O4/c1-3-5-7-8-9-11-16-25-21(23)19-14-12-13-18(17-19)20(22)24-15-1
InchiKey: RMMPZLFGCYWWTK-UHFFFAOYSA-N
Formula: C21H30O4
SMILES: C=CCCCOC(=O)c1cccc(C(=O)OCCCCCCCCC)c1
Mol. weight [g/mol]: 346.46

Physical Properties

Property code	Value	Unit	Source
gf	-151.28	kJ/mol	Joback Method
hf	-615.88	kJ/mol	Joback Method
hfus	48.09	kJ/mol	Joback Method
hvap	82.92	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.327		Crippen Method
mcvol	293.570	ml/mol	McGowan Method
pc	1290.21	kPa	Joback Method
rinpol	2549.00		NIST Webbook
tb	860.80	K	Joback Method
tc	1063.09	K	Joback Method
tf	507.93	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.38	J/mol×K	860.80	Joback Method
cpg	925.25	J/mol×K	894.51	Joback Method
cpg	939.98	J/mol×K	928.23	Joback Method
cpg	953.61	J/mol×K	961.94	Joback Method
cpg	966.16	J/mol×K	995.66	Joback Method
cpg	977.66	J/mol×K	1029.37	Joback Method
cpg	988.15	J/mol×K	1063.09	Joback Method
dvisc	0.0005479	Pa×s	507.93	Joback Method
dvisc	0.0003004	Pa×s	566.74	Joback Method

dvisc	0.0001844	Pa×s	625.55	Joback Method
dvisc	0.0001231	Pa×s	684.37	Joback Method
dvisc	0.0000876	Pa×s	743.18	Joback Method
dvisc	0.0000656	Pa×s	801.99	Joback Method
dvisc	0.0000510	Pa×s	860.80	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=U356718&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