Isophthalic acid, heptyl hex-2-yl ester

Inchi: InChI=1S/C21H32O4/c1-4-6-8-9-10-15-24-20(22)18-13-11-14-19(16-18)21(23)25-17(3)1
InchiKey: HSCLHVGLJVZWHH-UHFFFAOYSA-N
Formula: C21H32O4
SMILES: CCCCCCCOC(=O)c1cccc(C(=O)OC(C)CCCC)c1
Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
gf	-241.56	kJ/mol	Joback Method
hf	-746.59	kJ/mol	Joback Method
hfus	45.85	kJ/mol	Joback Method
hvap	83.20	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	5.549		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1259.27	kPa	Joback Method
rinpol	2446.00		NIST Webbook
rinpol	2446.00		NIST Webbook
tb	863.68	K	Joback Method
tc	1066.32	K	Joback Method
tf	494.69	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.65	J/mol×K	863.68	Joback Method
cpg	954.09	J/mol×K	897.45	Joback Method
cpg	969.33	J/mol×K	931.23	Joback Method
cpg	983.39	J/mol×K	965.00	Joback Method
cpg	996.30	J/mol×K	998.77	Joback Method
cpg	1008.08	J/mol×K	1032.54	Joback Method
cpg	1018.76	J/mol×K	1066.32	Joback Method
dvisc	0.0006043	Pa×s	494.69	Joback Method

dvisc	0.0003060	Pa×s	556.19	Joback Method
dvisc	0.0001775	Pa×s	617.69	Joback Method
dvisc	0.0001136	Pa×s	679.18	Joback Method
dvisc	0.0000783	Pa×s	740.68	Joback Method
dvisc	0.0000571	Pa×s	802.18	Joback Method
dvisc	0.0000436	Pa×s	863.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356771&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

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