Isophthalic acid, hept-2-yl isohexyl ester

Inchi: InChI=1S/C21H32O4/c1-5-6-7-11-17(4)25-21(23)19-13-8-12-18(15-19)20(22)24-14-9-10
InchiKey: JPQPEAQTVSBMDJ-UHFFFAOYSA-N
Formula: C21H32O4
SMILES: CCCCCC(C)OC(=O)c1cccc(C(=O)OCCCC(C)C)c1
Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
gf	-244.00	kJ/mol	Joback Method
hf	-751.87	kJ/mol	Joback Method
hfus	42.33	kJ/mol	Joback Method
hvap	82.81	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.405		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1266.45	kPa	Joback Method
rinpol	2400.00		NIST Webbook
tb	863.24	K	Joback Method
tc	1067.43	K	Joback Method
tf	479.69	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.15	J/mol×K	863.24	Joback Method
cpg	1008.83	J/mol×K	1033.40	Joback Method
cpg	997.06	J/mol×K	999.37	Joback Method
cpg	984.13	J/mol×K	965.34	Joback Method
cpg	970.02	J/mol×K	931.30	Joback Method
cpg	954.70	J/mol×K	897.27	Joback Method
cpg	1019.48	J/mol×K	1067.43	Joback Method
dvisc	0.0000399	Pa×s	863.24	Joback Method
dvisc	0.0000531	Pa×s	799.32	Joback Method

dvisc	0.0000742	Pa×s	735.39	Joback Method
dvisc	0.0001106	Pa×s	671.47	Joback Method
dvisc	0.0001793	Pa×s	607.54	Joback Method
dvisc	0.0003257	Pa×s	543.62	Joback Method
dvisc	0.0006933	Pa×s	479.69	Joback Method

Sources

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=U356527&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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