Isophthalic acid, 2-formylphenyl pentyl ester

Inchi: InChI=1S/C20H20O5/c1-2-3-6-12-24-19(22)15-9-7-10-16(13-15)20(23)25-18-11-5-4-8-17
InchiKey: XPOQHUMREOKZES-UHFFFAOYSA-N
Formula: C20H20O5
SMILES: CCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2C=O)c1
Mol. weight [g/mol]: 340.37

Physical Properties

Property code	Value	Unit	Source
gf	-244.28	kJ/mol	Joback Method
hf	-581.19	kJ/mol	Joback Method
hfus	42.72	kJ/mol	Joback Method
hvap	91.02	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.065		Crippen Method
mcvol	261.590	ml/mol	McGowan Method
pc	1826.28	kPa	Joback Method
rinpol	2839.00		NIST Webbook
tb	921.56	K	Joback Method
tc	1149.36	K	Joback Method
tf	579.36	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.62	J/mol×K	921.56	Joback Method
cpg	802.54	J/mol×K	959.53	Joback Method
cpg	813.18	J/mol×K	997.49	Joback Method
cpg	822.57	J/mol×K	1035.46	Joback Method
cpg	830.75	J/mol×K	1073.43	Joback Method
cpg	837.75	J/mol×K	1111.40	Joback Method
cpg	843.60	J/mol×K	1149.36	Joback Method
dvisc	0.0004477	Pa×s	579.36	Joback Method
dvisc	0.0002777	Pa×s	636.39	Joback Method

dvisc	0.0001863	Pa×s	693.43	Joback Method
dvisc	0.0001329	Pa×s	750.46	Joback Method
dvisc	0.0000994	Pa×s	807.49	Joback Method
dvisc	0.0000772	Pa×s	864.53	Joback Method
dvisc	0.0000619	Pa×s	921.56	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=U344614&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