Isophthalic acid, 2-formylphenyl nonyl ester

Inchi: InChI=1S/C24H28O5/c1-2-3-4-5-6-7-10-16-28-23(26)19-13-11-14-20(17-19)24(27)29-22
InchiKey: RAKKQCUXLMYGQH-UHFFFAOYSA-N
Formula: C24H28O5
SMILES: CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2C=O)c1
Mol. weight [g/mol]: 396.48

Physical Properties

Property code	Value	Unit	Source
gf	-210.60	kJ/mol	Joback Method
hf	-663.75	kJ/mol	Joback Method
hfus	53.08	kJ/mol	Joback Method
hvap	99.93	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	5.626		Crippen Method
mcvol	317.950	ml/mol	McGowan Method
pc	1347.68	kPa	Joback Method
rinpol	3277.00		NIST Webbook
rinpol	3277.00		NIST Webbook
tb	1013.08	K	Joback Method
tc	1243.64	K	Joback Method
tf	624.44	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.68	J/mol×K	1013.08	Joback Method
cpg	1036.86	J/mol×K	1051.51	Joback Method
cpg	1047.61	J/mol×K	1089.93	Joback Method
cpg	1056.98	J/mol×K	1128.36	Joback Method
cpg	1065.02	J/mol×K	1166.79	Joback Method
cpg	1071.79	J/mol×K	1205.22	Joback Method
cpg	1077.32	J/mol×K	1243.64	Joback Method
dvisc	0.0002927	Pa×s	624.44	Joback Method

dvisc	0.0001738	Pa×s	689.21	Joback Method
dvisc	0.0001129	Pa×s	753.99	Joback Method
dvisc	0.0000785	Pa×s	818.76	Joback Method
dvisc	0.0000575	Pa×s	883.53	Joback Method
dvisc	0.0000440	Pa×s	948.31	Joback Method
dvisc	0.0000349	Pa×s	1013.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344617&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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