

Isophthalic acid, 2-formylphenyl isobutyl ester

Inchi:	InChI=1S/C19H18O5/c1-13(2)12-23-18(21)14-7-5-8-15(10-14)19(22)24-17-9-4-3-6-16(17)
InchiKey:	ZUWDWQBENZNVTO-UHFFFAOYSA-N
Formula:	C19H18O5
SMILES:	CC(C)COC(=O)c1cccc(C(=O)Oc2ccccc2C=O)c1
Mol. weight [g/mol]:	326.34

Physical Properties

Property code	Value	Unit	Source
gf	-255.14	kJ/mol	Joback Method
hf	-565.83	kJ/mol	Joback Method
hfus	36.61	kJ/mol	Joback Method
hvap	88.41	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	3.531		Crippen Method
mvol	247.500	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
rinpol	2685.00		NIST Webbook
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tb	898.24	K	Joback Method
tc	1130.30	K	Joback Method
tf	553.09	K	Joback Method
vc	0.943	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.18	J/molxK	898.24	Joback Method
cpg	746.11	J/molxK	936.92	Joback Method
cpg	756.73	J/molxK	975.59	Joback Method
cpg	766.09	J/molxK	1014.27	Joback Method
cpg	774.21	J/molxK	1052.94	Joback Method
cpg	781.12	J/molxK	1091.62	Joback Method
cpg	786.85	J/molxK	1130.30	Joback Method
dvisc	0.0005329	Paxs	553.09	Joback Method

dvisc	0.0003180	Paxs	610.62	Joback Method
dvisc	0.0002074	Paxs	668.14	Joback Method
dvisc	0.0001448	Paxs	725.66	Joback Method
dvisc	0.0001065	Paxs	783.19	Joback Method
dvisc	0.0000817	Paxs	840.72	Joback Method
dvisc	0.0000649	Paxs	898.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344612&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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