

Fumaric acid, di(2-formylphenyl) ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C18H12O6/c19-11-13-5-1-3-7-15(13)23-17(21)9-10-18(22)24-16-8-4-2-6-14(16)

JDSGIIPZBXOCKL-MDZDMXLPSA-N

C18H12O6

O=Cc1ccccc1OC(=O)C=CC(=O)Oc1ccccc1C=O

324.28

Physical Properties

Property code	Value	Unit	Source
gf	-280.42	kJ/mol	Joback Method
hf	-508.27	kJ/mol	Joback Method
hfus	40.03	kJ/mol	Joback Method
hvap	93.25	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	2.379		Crippen Method
mcvol	230.680	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
rinpol	2753.00		NIST Webbook
rinpol	2753.00		NIST Webbook
tb	928.62	K	Joback Method
tc	1168.44	K	Joback Method
tf	593.74	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.21	J/mol×K	928.62	Joback Method
cpg	664.41	J/mol×K	968.59	Joback Method
cpg	672.49	J/mol×K	1008.56	Joback Method
cpg	679.51	J/mol×K	1048.53	Joback Method
cpg	685.52	J/mol×K	1088.50	Joback Method
cpg	690.57	J/mol×K	1128.47	Joback Method
cpg	694.68	J/mol×K	1168.44	Joback Method
dvisc	0.0004986	Pa×s	593.74	Joback Method

dvisc	0.0003199	Pa×s	649.55	Joback Method
dvisc	0.0002201	Pa×s	705.37	Joback Method
dvisc	0.0001600	Pa×s	761.18	Joback Method
dvisc	0.0001215	Pa×s	816.99	Joback Method
dvisc	0.0000956	Pa×s	872.81	Joback Method
dvisc	0.0000774	Pa×s	928.62	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=U405858&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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