

Fumaric acid, di(2-methoxyphenyl) ester

Inchi:	InChI=1S/C18H16O6/c1-21-13-7-3-5-9-15(13)23-17(19)11-12-18(20)24-16-10-6-4-8-14(14)
InchiKey:	PPVUVHOLUCZOCO-VAWYXSNFSA-N
Formula:	C18H16O6
SMILES:	COc1ccccc1OC(=O)C=CC(=O)Oc1ccccc1OC
Mol. weight [g/mol]:	328.32

Physical Properties

Property code	Value	Unit	Source
gf	-291.38	kJ/mol	Joback Method
hf	-601.55	kJ/mol	Joback Method
hfus	37.83	kJ/mol	Joback Method
hvap	84.63	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	2.771		Crippen Method
mvol	239.280	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinpol	2605.00		NIST Webbook
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tb	876.14	K	Joback Method
tc	1108.48	K	Joback Method
tf	554.20	K	Joback Method
vc	0.891	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.34	J/molxK	876.14	Joback Method
cpg	739.41	J/molxK	1069.75	Joback Method
cpg	732.66	J/molxK	1031.03	Joback Method
cpg	724.58	J/molxK	992.31	Joback Method
cpg	715.17	J/molxK	953.59	Joback Method
cpg	704.43	J/molxK	914.86	Joback Method
cpg	744.85	J/molxK	1108.48	Joback Method
dvisc	0.0000371	Paxs	876.14	Joback Method

dvisc	0.0000461	Paxs	822.48	Joback Method
dvisc	0.0000592	Paxs	768.83	Joback Method
dvisc	0.0000787	Paxs	715.17	Joback Method
dvisc	0.0001097	Paxs	661.51	Joback Method
dvisc	0.0001621	Paxs	607.86	Joback Method
dvisc	0.0002583	Paxs	554.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405944&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
mccvol:	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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