

Fumaric acid, ethyl 4-phenylphenyl ester

Inchi:	InChI=1S/C18H16O4/c1-2-21-17(19)12-13-18(20)22-16-10-8-15(9-11-16)14-6-4-3-5-7-14
InchiKey:	NQVLMHVHROWIGB-OUKQBFOZSA-N
Formula:	C18H16O4
SMILES:	CCOC(=O)C=CC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	296.32

Physical Properties

Property code	Value	Unit	Source
gf	-71.75	kJ/mol	Joback Method
hf	-325.64	kJ/mol	Joback Method
hfus	35.84	kJ/mol	Joback Method
hvap	79.15	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.378		Crippen Method
mcvol	227.540	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinqol	2501.00		NIST Webbook
tb	826.32	K	Joback Method
tc	1062.33	K	Joback Method
tf	497.22	K	Joback Method
vc	0.856	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.64	J/molxK	826.32	Joback Method
cpg	697.45	J/molxK	1022.99	Joback Method
cpg	688.48	J/molxK	983.66	Joback Method
cpg	678.47	J/molxK	944.32	Joback Method
cpg	667.36	J/molxK	904.99	Joback Method
cpg	655.10	J/molxK	865.65	Joback Method
cpg	705.44	J/molxK	1062.33	Joback Method
dvisc	0.0000639	Paxs	826.32	Joback Method
dvisc	0.0000808	Paxs	771.47	Joback Method

dvisc	0.0001060	Paxs	716.62	Joback Method
dvisc	0.0001455	Paxs	661.77	Joback Method
dvisc	0.0002113	Paxs	606.92	Joback Method
dvisc	0.0003305	Paxs	552.07	Joback Method
dvisc	0.0005707	Paxs	497.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348206&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

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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