

Fumaric acid, 4-phenylphenyl propyl ester

Inchi:	InChI=1S/C19H18O4/c1-2-14-22-18(20)12-13-19(21)23-17-10-8-16(9-11-17)15-6-4-3-5-7
InchiKey:	IVXJXGMTLBQHPP-OUKQBFOZSA-N
Formula:	C19H18O4
SMILES:	CCCOC(=O)C=CC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	310.34

Physical Properties

Property code	Value	Unit	Source
gf	-63.33	kJ/mol	Joback Method
hf	-346.28	kJ/mol	Joback Method
hfus	38.43	kJ/mol	Joback Method
hvap	81.37	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	3.768		Crippen Method
mcvol	241.630	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	2615.00		NIST Webbook
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tb	849.20	K	Joback Method
tc	1081.86	K	Joback Method
tf	508.49	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	697.45	J/molxK	849.20	Joback Method
cpg	754.15	J/molxK	1043.08	Joback Method
cpg	745.00	J/molxK	1004.31	Joback Method
cpg	734.81	J/molxK	965.53	Joback Method
cpg	723.53	J/molxK	926.75	Joback Method
cpg	711.09	J/molxK	887.98	Joback Method
cpg	762.32	J/molxK	1081.86	Joback Method
dvisc	0.0000560	Paxs	849.20	Joback Method

dvisc	0.0000712	Paxs	792.41	Joback Method
dvisc	0.0000937	Paxs	735.63	Joback Method
dvisc	0.0001293	Paxs	678.85	Joback Method
dvisc	0.0001891	Paxs	622.06	Joback Method
dvisc	0.0002985	Paxs	565.27	Joback Method
dvisc	0.0005219	Paxs	508.49	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=U348207&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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