

Fumaric acid, di(2-ethylphenyl) ester

Inchi:	InChI=1S/C20H20O4/c1-3-15-9-5-7-11-17(15)23-19(21)13-14-20(22)24-18-12-8-6-10-16
InchiKey:	REHWMOHIUJQLAP-BUHFOSPRSA-N
Formula:	C20H20O4
SMILES:	CCc1ccccc1OC(=O)C=CC(=O)Oc1ccccc1CC
Mol. weight [g/mol]:	324.37

Physical Properties

Property code	Value	Unit	Source
gf	-64.54	kJ/mol	Joback Method
hf	-378.39	kJ/mol	Joback Method
hfus	40.64	kJ/mol	Joback Method
hvap	84.26	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	3.879		Crippen Method
mcvol	255.720	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	2455.00		NIST Webbook
tb	877.06	K	Joback Method
tc	1107.75	K	Joback Method
tf	532.28	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.87	J/molxK	877.06	Joback Method
cpg	766.57	J/molxK	915.51	Joback Method
cpg	779.05	J/molxK	953.96	Joback Method
cpg	790.37	J/molxK	992.41	Joback Method
cpg	800.57	J/molxK	1030.85	Joback Method
cpg	809.71	J/molxK	1069.30	Joback Method
cpg	817.84	J/molxK	1107.75	Joback Method
dvisc	0.0004152	Paxs	532.28	Joback Method
dvisc	0.0002455	Paxs	589.74	Joback Method

dvisc	0.0001593	Paxs	647.21	Joback Method
dvisc	0.0001110	Paxs	704.67	Joback Method
dvisc	0.0000816	Paxs	762.13	Joback Method
dvisc	0.0000627	Paxs	819.60	Joback Method
dvisc	0.0000498	Paxs	877.06	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348801&Units=SI

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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