

Fumaric acid, isobutyl 4-phenylphenyl ester

Inchi:	InChI=1S/C20H20O4/c1-15(2)14-23-19(21)12-13-20(22)24-18-10-8-17(9-11-18)16-6-4-3
InchiKey:	BJOZXOHZSLCWDG-OUKQBFOZSA-N
Formula:	C20H20O4
SMILES:	CC(C)COC(=O)C=CC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	324.37

Physical Properties

Property code	Value	Unit	Source
gf	-57.35	kJ/mol	Joback Method
hf	-372.20	kJ/mol	Joback Method
hfus	37.50	kJ/mol	Joback Method
hvap	83.21	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.014		Crippen Method
mcvol	255.720	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinsol	2675.00		NIST Webbook
tb	871.64	K	Joback Method
tc	1104.81	K	Joback Method
tf	504.76	K	Joback Method
vc	0.962	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.65	J/molxK	871.64	Joback Method
cpg	812.43	J/molxK	1065.95	Joback Method
cpg	803.15	J/molxK	1027.09	Joback Method
cpg	792.80	J/molxK	988.22	Joback Method
cpg	781.30	J/molxK	949.36	Joback Method
cpg	768.61	J/molxK	910.50	Joback Method
cpg	820.69	J/molxK	1104.81	Joback Method
dvisc	0.0000448	Paxs	871.64	Joback Method
dvisc	0.0000579	Paxs	810.49	Joback Method

dvisc	0.0000780	Paxs	749.35	Joback Method
dvisc	0.0001109	Paxs	688.20	Joback Method
dvisc	0.0001686	Paxs	627.05	Joback Method
dvisc	0.0002808	Paxs	565.91	Joback Method
dvisc	0.0005291	Paxs	504.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348208&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
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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