Fumaric acid, isobutyl 2-propylphenyl ester

Inchi: InChI=1S/C17H22O4/c1-4-7-14-8-5-6-9-15(14)21-17(19)11-10-16(18)20-12-13(2)3/h5-6,
InchiKey: DEKPJOQHODOEHC-ZHACJKMWSA-N
Formula: C17H22O4
SMILES: CCCc1ccccc1OC(=O)C=CC(=O)OCC(C)C
Mol. weight [g/mol]: 290.35

Physical Properties

Property code	Value	Unit	Source
gf	-195.02	kJ/mol	Joback Method
hf	-546.81	kJ/mol	Joback Method
hfus	35.69	kJ/mol	Joback Method
hvap	74.26	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.300		Crippen Method
mcvol	237.210	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	2021.00		NIST Webbook
tb	776.32	K	Joback Method
tc	985.42	K	Joback Method
tf	444.53	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.89	J/mol×K	776.32	Joback Method
cpg	695.01	J/mol×K	811.17	Joback Method
cpg	709.10	J/mol×K	846.02	Joback Method
cpg	722.20	J/mol×K	880.87	Joback Method
cpg	734.32	J/mol×K	915.72	Joback Method
cpg	745.51	J/mol×K	950.57	Joback Method
cpg	755.77	J/mol×K	985.42	Joback Method
dvisc	0.0008333	Pa×s	444.53	Joback Method
dvisc	0.0004315	Pa×s	499.83	Joback Method

dvisc	0.0002548	Pa×s	555.13	Joback Method
dvisc	0.0001655	Pa×s	610.42	Joback Method
dvisc	0.0001155	Pa×s	665.72	Joback Method
dvisc	0.0000852	Pa×s	721.02	Joback Method
dvisc	0.0000656	Pa×s	776.32	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U348125&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