Fumaric acid, 2-ethylphenyl isobutyl ester

Inchi: InChI=1S/C16H20O4/c1-4-13-7-5-6-8-14(13)20-16(18)10-9-15(17)19-11-12(2)3/h5-10,12
InchiKey: KOGVAGQWEJCZMU-MDZDMXLPSA-N
Formula: C16H20O4
SMILES: CCc1ccccc1OC(=O)C=CC(=O)OCC(C)C
Mol. weight [g/mol]: 276.33

Physical Properties

Property code	Value	Unit	Source
gf	-203.44	kJ/mol	Joback Method
hf	-526.17	kJ/mol	Joback Method
hfus	33.10	kJ/mol	Joback Method
hvap	72.03	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.910		Crippen Method
mcvol	223.120	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
rinpol	1969.00		NIST Webbook
rinpol	1969.00		NIST Webbook
tb	753.44	K	Joback Method
tc	964.70	K	Joback Method
tf	433.26	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.51	J/mol×K	753.44	Joback Method
cpg	639.34	J/mol×K	788.65	Joback Method
cpg	653.17	J/mol×K	823.86	Joback Method
cpg	666.02	J/mol×K	859.07	Joback Method
cpg	677.92	J/mol×K	894.28	Joback Method
cpg	688.90	J/mol×K	929.49	Joback Method
cpg	698.98	J/mol×K	964.70	Joback Method
dvisc	0.0009089	Pa×s	433.26	Joback Method

dvisc	0.0004767	Pa×s	486.62	Joback Method
dvisc	0.0002840	Pa×s	539.99	Joback Method
dvisc	0.0001857	Pa×s	593.35	Joback Method
dvisc	0.0001303	Pa×s	646.71	Joback Method
dvisc	0.0000965	Pa×s	700.08	Joback Method
dvisc	0.0000745	Pa×s	753.44	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=U348798&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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