Fumaric acid, butyl 2-ethylphenyl ester

Inchi: InChI=1S/C16H20O4/c1-3-5-12-19-15(17)10-11-16(18)20-14-9-7-6-8-13(14)4-2/h6-11H,3
InchiKey: KSXSQWYDZYFTKX-ZHACJKMWSA-N
Formula: C16H20O4
SMILES: CCCCOC(=O)C=CC(=O)Oc1ccccc1CC
Mol. weight [g/mol]: 276.33

Physical Properties

Property code	Value	Unit	Source
gf	-201.00	kJ/mol	Joback Method
hf	-520.89	kJ/mol	Joback Method
hfus	36.62	kJ/mol	Joback Method
hvap	72.42	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.054		Crippen Method
mcvol	223.120	ml/mol	McGowan Method
pc	1900.26	kPa	Joback Method
rinpol	2020.00		NIST Webbook
tb	753.88	K	Joback Method
tc	961.93	K	Joback Method
tf	448.26	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.96	J/mol×K	753.88	Joback Method
cpg	687.57	J/mol×K	927.25	Joback Method
cpg	676.67	J/mol×K	892.58	Joback Method
cpg	664.89	J/mol×K	857.90	Joback Method
cpg	652.19	J/mol×K	823.23	Joback Method
cpg	638.55	J/mol×K	788.55	Joback Method
cpg	697.61	J/mol×K	961.93	Joback Method
dvisc	0.0000809	Pa×s	753.88	Joback Method
dvisc	0.0001030	Pa×s	702.94	Joback Method

dvisc	0.0001362	Pa×s	652.01	Joback Method
dvisc	0.0001887	Pa×s	601.07	Joback Method
dvisc	0.0002779	Pa×s	550.13	Joback Method
dvisc	0.0004428	Pa×s	499.20	Joback Method
dvisc	0.0007844	Pa×s	448.26	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=U348799&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

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