Fumaric acid, butyl 2-propylphenyl ester

Inchi: InChI=1S/C17H22O4/c1-3-5-13-20-16(18)11-12-17(19)21-15-10-7-6-9-14(15)8-4-2/h6-7,
InchiKey: CLXPPLNGQHQZBY-VAWYXSNFSA-N
Formula: C17H22O4
SMILES: CCCCOC(=O)C=CC(=O)Oc1ccccc1CCC
Mol. weight [g/mol]: 290.35

Physical Properties

Property code	Value	Unit	Source
gf	-192.58	kJ/mol	Joback Method
hf	-541.53	kJ/mol	Joback Method
hfus	39.21	kJ/mol	Joback Method
hvap	74.64	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.444		Crippen Method
mcvol	237.210	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	2067.00		NIST Webbook
rinpol	2067.00		NIST Webbook
tb	776.76	K	Joback Method
tc	982.95	K	Joback Method
tf	459.53	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.33	J/mol×K	776.76	Joback Method
cpg	694.24	J/mol×K	811.12	Joback Method
cpg	708.16	J/mol×K	845.49	Joback Method
cpg	721.12	J/mol×K	879.85	Joback Method
cpg	733.15	J/mol×K	914.22	Joback Method
cpg	744.26	J/mol×K	948.58	Joback Method
cpg	754.50	J/mol×K	982.95	Joback Method
dvisc	0.0007226	Pa×s	459.53	Joback Method

dvisc	0.0004025	Pa×s	512.40	Joback Method
dvisc	0.0002501	Pa×s	565.27	Joback Method
dvisc	0.0001686	Pa×s	618.14	Joback Method
dvisc	0.0001210	Pa×s	671.02	Joback Method
dvisc	0.0000911	Pa×s	723.89	Joback Method
dvisc	0.0000713	Pa×s	776.76	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=U348126&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