Fumaric acid, 1-phenylprop-1-yl 2-ethylhexyl ester

Inchi: InChI=1S/C21H30O4/c1-4-7-11-17(5-2)16-24-20(22)14-15-21(23)25-19(6-3)18-12-9-8-10

InchiKey: ZDSUNJXXKIDOOJ-CCEZHUSRSA-N

Formula: C21H30O4

SMILES: CCCCC(CC)COC(=O)C=CC(=O)OC(CC)c1ccccc1

Mol. weight [g/mol]: 346.46

Physical Properties

Property code	Value	Unit	Source
gf	-154.15	kJ/mol	Joback Method
hf	-623.18	kJ/mol	Joback Method
hfus	42.92	kJ/mol	Joback Method
hvap	82.11	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.997		Crippen Method
mcvol	293.570	ml/mol	McGowan Method
pc	1329.07	kPa	Joback Method
rinpol	2391.00		NIST Webbook
rinpol	2391.00		NIST Webbook
tb	862.42	K	Joback Method
tc	1069.82	K	Joback Method
tf	462.09	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.99	J/mol×K	862.42	Joback Method
cpg	928.20	J/mol×K	896.99	Joback Method
cpg	943.23	J/mol×K	931.55	Joback Method
cpg	957.15	J/mol×K	966.12	Joback Method
cpg	969.99	J/mol×K	1000.69	Joback Method
cpg	981.80	J/mol×K	1035.25	Joback Method
cpg	992.62	J/mol×K	1069.82	Joback Method
dvisc	0.0007804	Pa×s	462.09	Joback Method

dvisc	0.0003339	Pa×s	528.81	Joback Method
dvisc	0.0001728	Pa×s	595.53	Joback Method
dvisc	0.0001021	Pa×s	662.25	Joback Method
dvisc	0.0000664	Pa×s	728.98	Joback Method
dvisc	0.0000465	Pa×s	795.70	Joback Method
dvisc	0.0000343	Pa×s	862.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405902&Units=SI
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

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