Fumaric acid, 2-phenethyl 2-ethylhexyl ester

Inchi: InChI=1S/C20H28O4/c1-3-5-9-17(4-2)16-24-20(22)13-12-19(21)23-15-14-18-10-7-6-8-11
InchiKey: DDSRMVJVDCAOEG-OUKQBFOZSA-N
Formula: C20H28O4
SMILES: CCCCC(CC)COC(=O)C=CC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 332.43

Physical Properties

Property code	Value	Unit	Source
gf	-160.13	kJ/mol	Joback Method
hf	-597.26	kJ/mol	Joback Method
hfus	43.85	kJ/mol	Joback Method
hvap	80.27	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.088		Crippen Method
mcvol	279.480	ml/mol	McGowan Method
pc	1418.64	kPa	Joback Method
rinpol	2401.00		NIST Webbook
rinpol	2401.00		NIST Webbook
tb	839.98	K	Joback Method
tc	1045.27	K	Joback Method
tf	465.82	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.53	J/mol×K	839.98	Joback Method
cpg	868.41	J/mol×K	874.19	Joback Method
cpg	883.19	J/mol×K	908.41	Joback Method
cpg	896.90	J/mol×K	942.62	Joback Method
cpg	909.59	J/mol×K	976.84	Joback Method
cpg	921.29	J/mol×K	1011.05	Joback Method
cpg	932.05	J/mol×K	1045.27	Joback Method
dvisc	0.0007457	Pa×s	465.82	Joback Method

dvisc	0.0003506	Pa×s	528.18	Joback Method
dvisc	0.0001933	Pa×s	590.54	Joback Method
dvisc	0.0001194	Pa×s	652.90	Joback Method
dvisc	0.0000802	Pa×s	715.26	Joback Method
dvisc	0.0000575	Pa×s	777.62	Joback Method
dvisc	0.0000432	Pa×s	839.98	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=U405681&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