Fumaric acid, ethyl 4-phenoxybenzyl ester

Inchi: InChI=1S/C19H18O5/c1-2-22-18(20)12-13-19(21)23-14-15-8-10-17(11-9-15)24-16-6-4-3
InchiKey: LKGNHRKJPOLBBK-OUKQBFOZSA-N
Formula: C19H18O5
SMILES: CCOC(=O)C=CC(=O)OCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 326.34

Physical Properties

Property code	Value	Unit	Source
gf	-168.33	kJ/mol	Joback Method
hf	-478.50	kJ/mol	Joback Method
hfus	39.62	kJ/mol	Joback Method
hvap	83.78	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.641		Crippen Method
mcvol	247.500	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
rinpol	2500.00		NIST Webbook
rinpol	2500.00		NIST Webbook
tb	871.62	K	Joback Method
tc	1102.40	K	Joback Method
tf	530.72	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.94	J/mol×K	871.62	Joback Method
cpg	736.93	J/mol×K	910.08	Joback Method
cpg	748.66	J/mol×K	948.55	Joback Method
cpg	759.15	J/mol×K	987.01	Joback Method
cpg	768.44	J/mol×K	1025.47	Joback Method
cpg	776.57	J/mol×K	1063.93	Joback Method
cpg	783.58	J/mol×K	1102.40	Joback Method
dvisc	0.0003720	Pa×s	530.72	Joback Method

dvisc	0.0002173	Pa×s	587.54	Joback Method
dvisc	0.0001396	Pa×s	644.35	Joback Method
dvisc	0.0000963	Pa×s	701.17	Joback Method
dvisc	0.0000703	Pa×s	757.99	Joback Method
dvisc	0.0000536	Pa×s	814.80	Joback Method
dvisc	0.0000423	Pa×s	871.62	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=U348109&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