Fumaric acid, 2-phenethyl hept-2-yl ester

Inchi: InChI=1S/C19H26O4/c1-3-4-6-9-16(2)23-19(21)13-12-18(20)22-15-14-17-10-7-5-8-11-17
InchiKey: NAZVGKODDTWYIY-OUKQBFOZSA-N
Formula: C19H26O4
SMILES: CCCCCC(C)OC(=O)C=CC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	-168.55	kJ/mol	Joback Method
hf	-576.62	kJ/mol	Joback Method
hfus	41.26	kJ/mol	Joback Method
hvap	78.05	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.841		Crippen Method
mcvol	265.390	ml/mol	McGowan Method
pc	1527.07	kPa	Joback Method
rinpol	2282.00		NIST Webbook
tb	817.10	K	Joback Method
tc	1022.78	K	Joback Method
tf	454.55	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.38	J/mol×K	817.10	Joback Method
cpg	862.35	J/mol×K	988.50	Joback Method
cpg	850.77	J/mol×K	954.22	Joback Method
cpg	838.22	J/mol×K	919.94	Joback Method
cpg	824.66	J/mol×K	885.66	Joback Method
cpg	810.06	J/mol×K	851.38	Joback Method
cpg	873.00	J/mol×K	1022.78	Joback Method
dvisc	0.0000497	Pa×s	817.10	Joback Method
dvisc	0.0000659	Pa×s	756.67	Joback Method

dvisc	0.0000918	Pa×s	696.25	Joback Method
dvisc	0.0001360	Pa×s	635.82	Joback Method
dvisc	0.0002190	Pa×s	575.40	Joback Method
dvisc	0.0003943	Pa×s	514.98	Joback Method
dvisc	0.0008301	Pa×s	454.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405679&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