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

Inchi: InChI=1S/C20H28O4/c1-4-6-8-11-16(3)23-19(21)14-15-20(22)24-18(5-2)17-12-9-7-10-13
InchiKey: GOARFDBVBNKNEN-CCEZHUSRSA-N
Formula: C20H28O4
SMILES: CCCCCC(C)OC(=O)C=CC(=O)OC(CC)c1ccccc1
Mol. weight [g/mol]: 332.43

Physical Properties

Property code	Value	Unit	Source
gf	-162.57	kJ/mol	Joback Method
hf	-602.54	kJ/mol	Joback Method
hfus	40.33	kJ/mol	Joback Method
hvap	79.88	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.749		Crippen Method
mcvol	279.480	ml/mol	McGowan Method
pc	1427.22	kPa	Joback Method
rinpol	2275.00		NIST Webbook
rinpol	2275.00		NIST Webbook
tb	839.54	K	Joback Method
tc	1046.97	K	Joback Method
tf	450.82	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.05	J/mol×K	839.54	Joback Method
cpg	922.25	J/mol×K	1012.40	Joback Method
cpg	910.52	J/mol×K	977.83	Joback Method
cpg	897.78	J/mol×K	943.26	Joback Method
cpg	883.99	J/mol×K	908.68	Joback Method
cpg	869.09	J/mol×K	874.11	Joback Method
cpg	933.00	J/mol×K	1046.97	Joback Method
dvisc	0.0000396	Pa×s	839.54	Joback Method

dvisc	0.0000535	Pa×s	774.75	Joback Method
dvisc	0.0000764	Pa×s	709.97	Joback Method
dvisc	0.0001170	Pa×s	645.18	Joback Method
dvisc	0.0001971	Pa×s	580.39	Joback Method
dvisc	0.0003786	Pa×s	515.61	Joback Method
dvisc	0.0008773	Pa×s	450.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405900&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