Fumaric acid, 4-methoxyphenyl hept-2-yl ester

Inchi: InChI=1S/C18H24O5/c1-4-5-6-7-14(2)22-17(19)12-13-18(20)23-16-10-8-15(21-3)9-11-16
InchiKey: KYPMHSBPMAMSKD-OUKQBFOZSA-N
Formula: C18H24O5
SMILES: CCCCCC(C)OC(=O)C=CC(=O)Oc1ccc(OC)cc1
Mol. weight [g/mol]: 320.38

Physical Properties

Property code	Value	Unit	Source
gf	-291.60	kJ/mol	Joback Method
hf	-699.67	kJ/mol	Joback Method
hfus	39.47	kJ/mol	Joback Method
hvap	78.89	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.669		Crippen Method
mcvol	257.170	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinpol	2360.00		NIST Webbook
rinpol	2360.00		NIST Webbook
tb	821.62	K	Joback Method
tc	1028.71	K	Joback Method
tf	478.03	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.47	J/mol×K	821.62	Joback Method
cpg	779.39	J/mol×K	856.14	Joback Method
cpg	793.20	J/mol×K	890.65	Joback Method
cpg	805.93	J/mol×K	925.17	Joback Method
cpg	817.60	J/mol×K	959.68	Joback Method
cpg	828.21	J/mol×K	994.20	Joback Method
cpg	837.79	J/mol×K	1028.71	Joback Method
dvisc	0.0005308	Pa×s	478.03	Joback Method

dvisc	0.0002798	Pa×s	535.29	Joback Method
dvisc	0.0001670	Pa×s	592.56	Joback Method
dvisc	0.0001091	Pa×s	649.82	Joback Method
dvisc	0.0000764	Pa×s	707.09	Joback Method
dvisc	0.0000564	Pa×s	764.35	Joback Method
dvisc	0.0000435	Pa×s	821.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405780&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